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Supplementary Information

Three-component synthesis of arylsulfonyl-substituted indolo[2,1-a]isoquinolinones and benzimidazo-[2,1-*a*]isoquinolin-6(5*H*)-ones by SO_2 insertion and radical cascade cyclization

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1. General Considerations

Unless otherwise noted, all chemicals were purchased and used without further purifications. ^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature on a 300 or 400 MHz NMR spectrometer (75 or 100 MHz for ^{13}C). NMR experiments are reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$ (7.26 or 77.0 ppm) as the internal standard. The coupling constants *J* are given in Hz. Column chromatography was performed using EM Silica gel 60 (300-400 mesh).

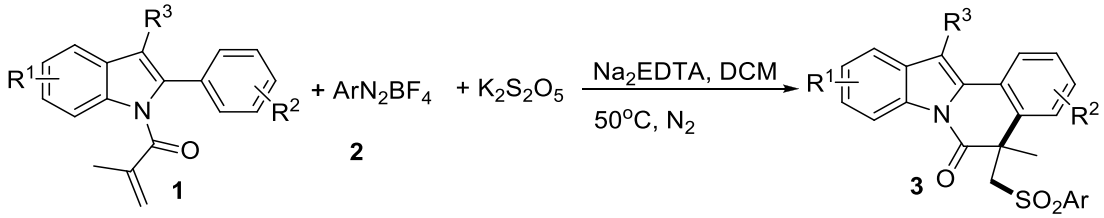
2. General Synthetic Procedures

The synthesis of 2-arylindoles 1: The substrate 2-arylindoles (**1**) were synthesized from arylhydrazine hydrochlorides and ketones according to the literature.[1]

The synthesis of aryldiazonium tetrafluoroborate 2: Aryldiazonium tetrafluoroborates were synthesized from commercially available anilines according to the literature.[2] After the completion of the reaction, the residue was used directly without further purifications.

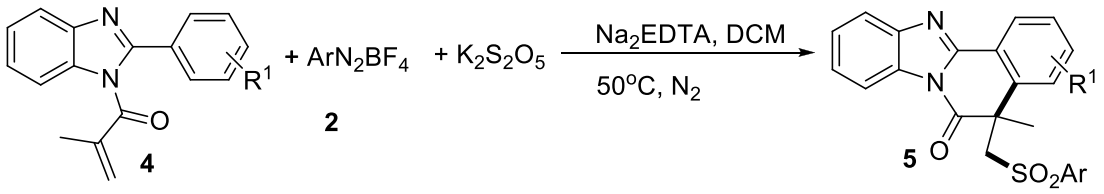
The synthesis of 2-arylbenzimidazole 4： The 2-arylbenzimidazoles (**4**) were synthesized from benzimidazoles and methacryloyl chlorides according to the literature.[3]

Typical procedure for the synthesis of product 3:



Under N_2, a 10 mL Schlenk tube equipped with a stir bar was charged with **1** (0.2 mmol), **2** (0.3 mmol, 1.5 equiv.), $K_2S_2O_5$ (0.4 mmol, 88 mg, 2 equiv.), Na_2EDTA (0.2 mmol, 74.4 mg, 1 equiv.), DCM (2 mL) and sealed. The reaction mixture was stirred at 50 ℃ for 12 h in oil bath. After removing of volatile materials from the reaction mixture under vacuum, the resulted residue was purified by flash column chromatography on silica gel to give the corresponding arylsulfonyl indolo[2,1-*a*]isoquinolin-6(5*H*)-one **3**.

Typical procedure for the synthesis of product 5:



Under N_2, a 10 mL Schlenk tube equipped with a stir bar was charged with **4** (0.2 mmol), **2** (0.3 mmol, 1.5 equiv.), $K_2S_2O_5$ (0.4 mmol, 88 mg, 2 equiv.), Na_2EDTA (0.2 mmol, 74.4 mg, 1 equiv.), DCM (2 mL) and sealed. The reaction mixture was stirred at 50 ℃ for 12 h in oil bath. After removing of volatile materials from the reaction mixture under vacuum, the resulted residue

was purified by flash column chromatography on silica gel to give the corresponding arylsulfonyl-substituted benzimidazo-[2,1-*a*]isoquinolin-6(5*H*)-ones (**5**).

3. Radical inhibition and trapping experiments

Under N_2, a 10 mL Schlenk tube equipped with a stir bar was charged with **1a** (0.2 mmol), **2a** (1.5 equiv.), $K_2S_2O_5$ (2 equiv.), Na_2EDTA (1 equiv.), TEMPO (2.0 equiv.), DCM (2 mL) and sealed. The reaction mixture was stirred at 50 ℃ for 12 h in oil bath. The reaction was completely inhibited without the detection of product **3aa**.

Under N_2, a 10 mL Schlenk tube equipped with a stir bar was charged with **1a** (0.2 mmol), **2a** (1.5 eq), $K_2S_2O_5$ (2 equiv.), Na_2EDTA (1 equiv.), TEMPO (2.0 equiv.), 1,1-diphenylethylene (3.0 equiv.), DCM (2 mL) and sealed. The reaction mixture was stirred at 50 ℃ for 12 h in oil bath. The yield of **3aa** is decreased to 35%, along with the formation of adduct **6** and **7**.

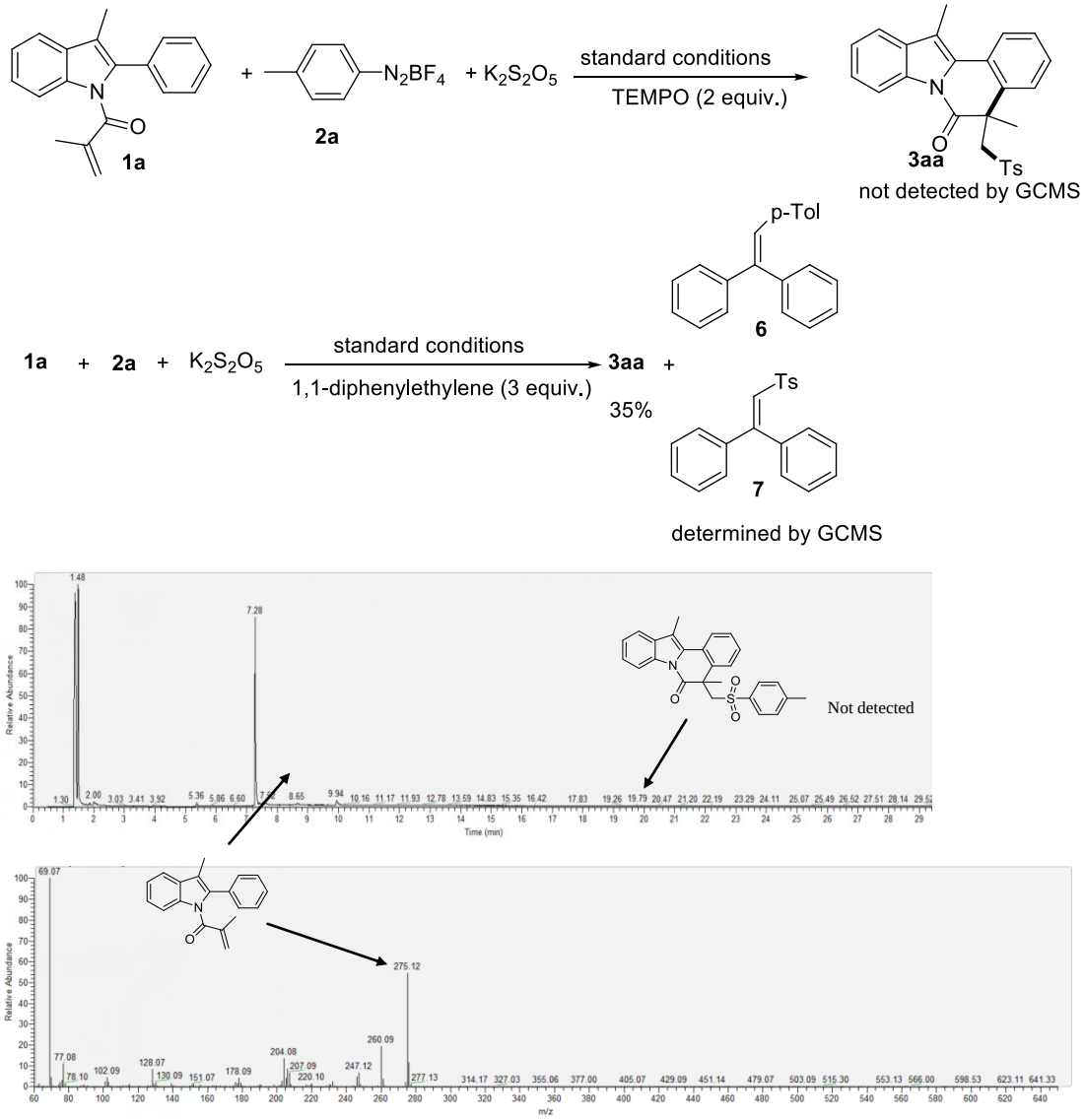


Figure S1 GCMS spectra of the reaction mixture by adding 2 equivalents of TEMPO.

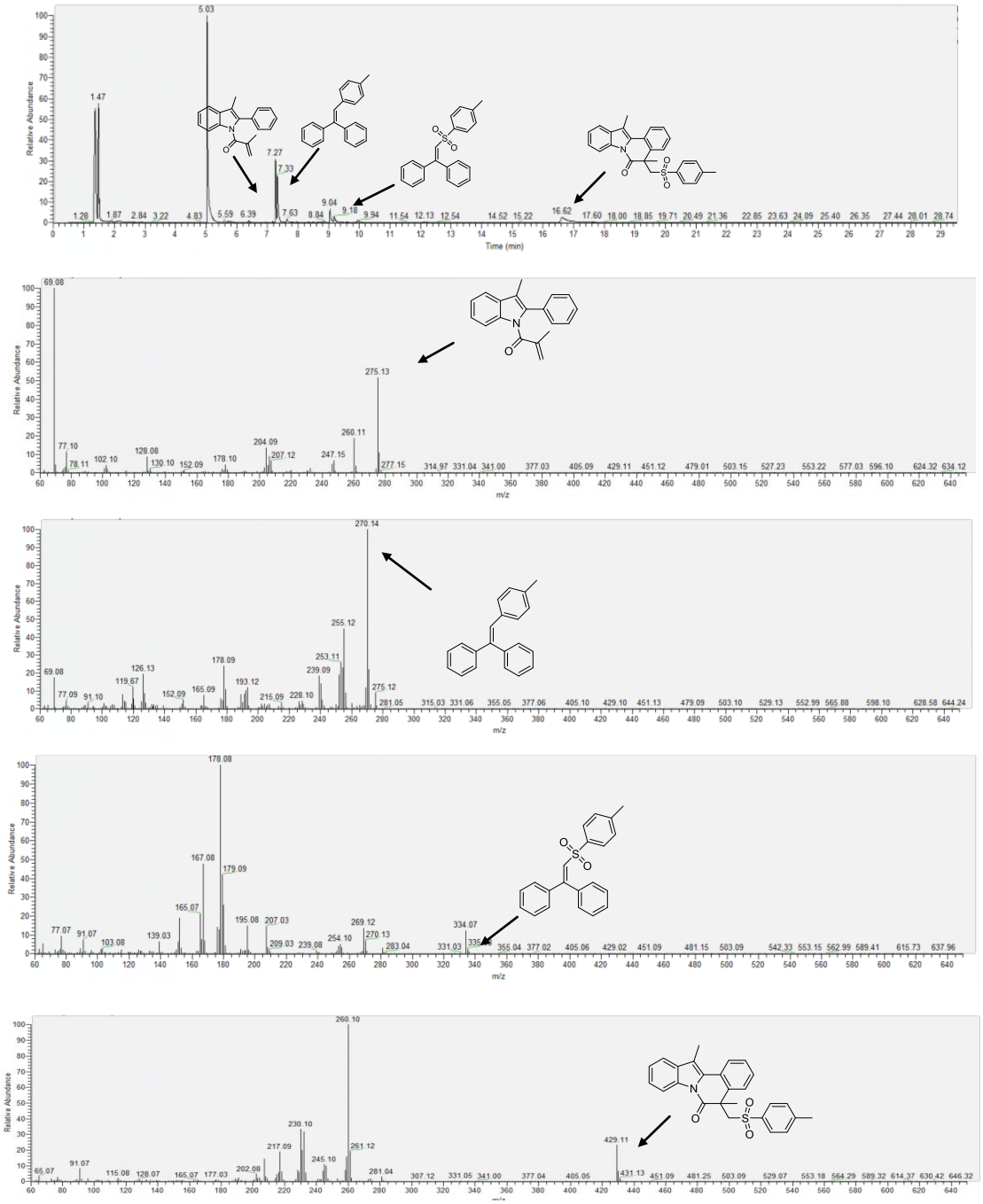
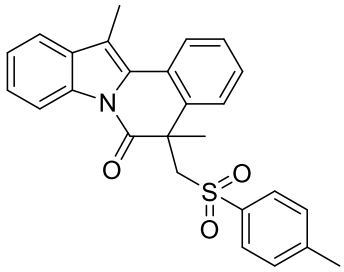


Figure S2 GCMS spectra of the reaction mixture by adding 3 equivalents of 1,1-diphenylethylene.

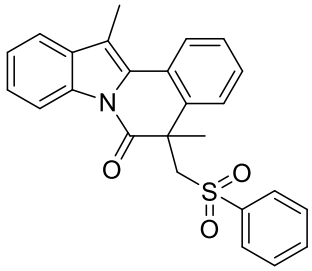
4. Characterization Data for the Products

5,12-Dimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3aa)[4]



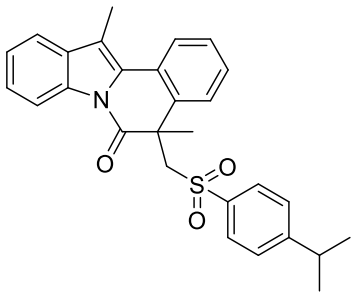
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3aa** (76%, white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.58 (m, 1H), 7.41 – 7.30 (m, 6H), 7.21 (t, *J* = 7.6 Hz, 1H), 6.96 (d, *J* = 7.9 Hz, 2H), 4.57 (d, *J* = 14.6 Hz, 1H), 3.95 (d, *J* = 14.6 Hz, 1H), 2.67 (s, 3H), 2.14 (s, 3H), 1.62 (s, 3H).

5,12-Dimethyl-5-((phenylsulfonyl)methyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ab)



Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ab** (79%, yellow solid). mp 171-173 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.47 – 8.44 (m, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.54 – 7.49 (m, 1H), 7.45 – 7.43 (m, 2H), 7.34 – 7.26 (m, 4H), 7.20 – 7.16 (m, 3H), 7.09 (t, *J* = 7.4 Hz, 1H), 4.51 (d, *J* = 14.4 Hz, 1H), 3.89 (d, *J* = 14.6 Hz, 1H), 2.60 (s, 3H), 1.55 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 140.3, 134.3, 134.3, 133.2, 132.5, 129.3, 128.8, 127.9, 127.7, 127.5, 127.1, 126.3, 125.8, 125.2, 124.4, 118.5, 117.0, 115.1, 64.4, 46.6, 31.7, 11.7. HRMS (ESI) *m/z* calcd for $C_{25}H_{22}NO_3S$ [M+H$^+$]: 416.1315, found 416.1314.

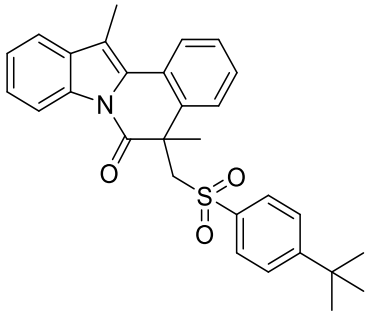
5-(((4-Isopropylphenyl)sulfonyl)methyl)-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ac)



Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ac** (83%, white solid). mp 198-199 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.43 (m, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.48 (m, 1H), 7.31 – 7.24 (m, 5H), 7.16 – 7.14 (m, 1H), 7.05 – 7.02 (m,

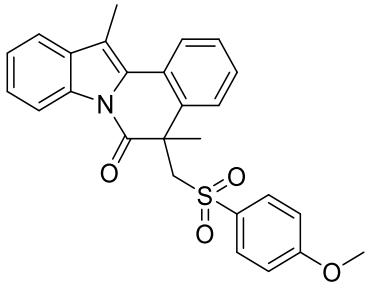
1H), 6.97 (d, *J* = 8.2 Hz, 2H), 4.49 (d, *J* = 14.6 Hz, 1H), 3.87 (d, *J* = 14.7 Hz, 1H), 2.73 – 2.62 (m, 1H), 2.57 (s, 3H), 1.52 (s, 3H), 1.05 – 1.02 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 154.8, 137.3, 134.3, 134.2, 132.4, 129.3, 128.0, 127.8, 127.4, 127.3, 126.9, 126.3, 125.8, 125.1, 124.4, 118.5, 116.9, 115.0, 64.4, 46.5, 34.1, 31.8, 23.6, 23.5, 11.7. HRMS (ESI) *m/z* calcd for $C_{28}H_{28}NO_3S$ [M+H$^+$]: 458.1784, found 458.1785.

5-(((4-(Tert-butyl)phenyl)sulfonyl)methyl)-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ad)



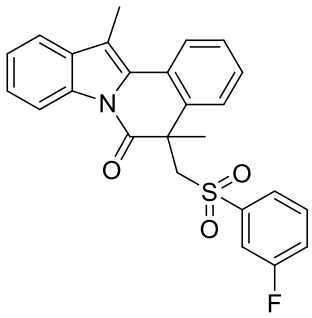
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ad** (75%, yellow solid). mp 205-207 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.43 (m, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.49 (m, 1H), 7.31 – 7.25 (m, 5H), 7.18 – 7.13 (m, 3H), 7.05 (t, *J* = 7.6 Hz, 1H), 4.51 (d, *J* = 14.6 Hz, 1H), 3.88 (d, *J* = 14.6 Hz, 1H), 2.58 (s, 3H), 1.52 (s, 3H), 1.11 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 157.1, 136.9, 134.3, 134.2, 132.4, 129.3, 127.8, 127.7, 127.4, 127.3, 126.3, 125.9, 125.8, 125.1, 124.4, 118.5, 116.9, 115.0, 64.3, 46.6, 35.1, 31.9, 30.9, 11.7. HRMS (ESI) *m/z* calcd for $C_{29}H_{30}NO_3S$ [M+H$^+$]: 472.1941, found 472.1943.

5-(((4-Methoxyphenyl)sulfonyl)methyl)-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-on (3ae)



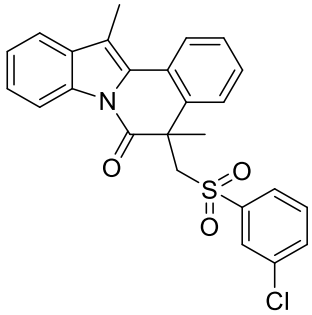
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ae** (70%, yellow oil). mp 151-152 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 – 8.37 (m, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.49 (m, 1H), 7.34 – 7.24 (m, 6H), 7.19 – 7.15 (m, 1H), 6.50 (d, *J* = 8.6 Hz, 2H), 4.49 (d, *J* = 14.6 Hz, 1H), 3.85 (d, *J* = 14.6 Hz, 1H), 3.50 (s, 3H), 2.58 (s, 3H), 1.53 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 163.3, 134.3, 134.3, 132.4, 130.9, 130.1, 129.3, 127.8, 127.6, 127.5, 126.2, 125.8, 125.1, 124.4, 118.4, 116.9, 115.0, 113.8, 64.6, 55.4, 46.4, 32.0, 11.7. HRMS (ESI) *m/z* calcd for $C_{26}H_{24}NO_4S$ [M+H$^+$]: 446.1421, found 446.1420.

5-(((3-Fluorophenyl)sulfonyl)methyl)-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3af)



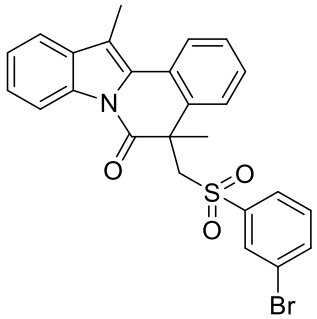
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3af** (68%, yellow solid). mp 180-182 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 – 8.45 (m, 1H), 7.95 (d, *J* = 8.1 Hz, 1H), 7.52 – 7.50 (m, 1H), 7.31 – 7.23 (m, 4H), 7.17 – 7.10 (m, 2H), 7.05 – 6.99 (m, 2H), 6.97 – 6.92 (m, 1H), 4.50 (d, *J* = 14.7 Hz, 1H), 3.88 (d, *J* = 14.8 Hz, 1H), 2.58 (s, 3H), 1.54 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.1, 162.0 (d, J_{C-F} = 250.4 Hz), 142.1 (d, J_{C-F} = 6.5 Hz), 134.3, 134.0, 132.4, 130.7 (d, J_{C-F} = 7.6 Hz), 129.1, 128.0, 127.4, 127.1, 126.4, 126.0, 125.2, 124.5, 123.6 (d, J_{C-F} = 3.3 Hz), 120.5 (d, J_{C-F} = 21.1 Hz), 118.6, 116.9, 115.4, 115.2 (d, J_{C-F} = 24.4 Hz), 64.6, 46.5, 31.5, 11.7. HRMS (ESI) *m/z* calcd for $C_{25}H_{21}FNO_3S$ [M+H$^+$]: 434.1221, found 434.1223.

5-(((3-Chlorophenyl)sulfonyl)methyl)-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ag)



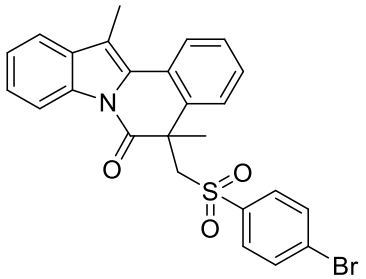
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ag** (80%, white solid). mp 191-193 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 – 8.44 (m, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.53 – 7.51 (m, 1H), 7.36 – 7.28 (m, 4H), 7.23 – 7.17 (m, 2H), 7.13 – 7.03 (m, 3H), 4.52 (d, *J* = 14.7 Hz, 1H), 3.89 (d, *J* = 14.8 Hz, 1H), 2.60 (s, 3H), 1.56 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 141.5, 134.9, 134.3, 133.8, 133.4, 132.4, 130.1, 129.1, 128.1, 128.1, 127.4, 127.1, 126.4, 126.0, 126.0, 125.1, 124.6, 118.6, 116.9, 115.5, 64.7, 46.4, 31.6, 11.7. HRMS (ESI) *m/z* calcd for $C_{25}H_{21}ClNO_3S$ [M+H$^+$]: 450.0925, found 450.0923.

5-(((3-Bromophenyl)sulfonyl)methyl)-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ah)



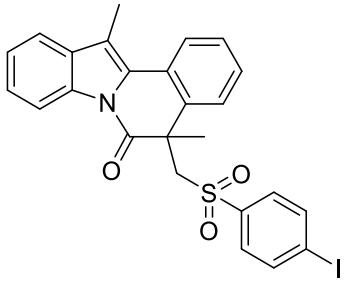
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ah** (62%, yellow solid). mp 219-221 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 – 8.55 (m, 1H), 8.07 (d, *J* = 8.1 Hz, 1H), 7.62 – 7.60 (m, 1H), 7.49 – 7.46 (m, 1H), 7.44 – 7.36 (m, 5H), 7.19 – 7.16 (m, 1H), 7.13 – 7.08 (m, 2H), 4.60 (d, *J* = 14.7 Hz, 1H), 3.98 (d, *J* = 14.8 Hz, 1H), 2.69 (s, 3H), 1.64 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 141.6, 136.3, 134.3, 133.7, 132.4, 130.9, 130.3, 129.1, 128.2, 127.4, 127.1, 126.4, 126.4, 126.0, 125.2, 124.6, 122.7, 118.6, 116.9, 115.5, 64.6, 46.4, 31.6, 11.8. HRMS (ESI) *m/z* calcd for $C_{25}H_{21}BrNO_3S$ [M+H$^+$]: 499.0420, found 499.0422.

5-(((4-Bromophenyl)sulfonyl)methyl)-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ai)



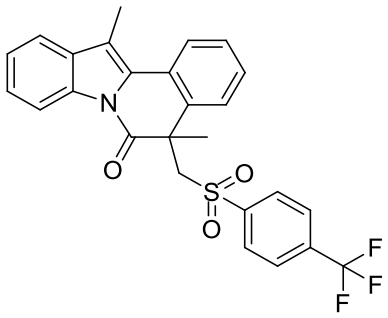
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ai** (65%, yellow solid). mp 207-209 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.39 (m, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.50 – 7.48 (m, 1H), 7.32 – 7.24 (m, 3H), 7.23 – 7.17 (m, 4H), 7.14 – 7.11 (m, 1H), 7.08 – 7.04 (m, 1H), 4.45 (d, *J* = 14.7 Hz, 1H), 3.85 (d, *J* = 14.7 Hz, 1H), 2.55 (s, 3H), 1.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 138.9, 134.2, 134.1, 132.4, 132.0, 129.4, 129.1, 128.8, 127.9, 127.6, 127.2, 126.3, 126.1, 125.2, 124.6, 118.6, 116.9, 115.4, 64.5, 46.5, 31.7, 11.7. HRMS (ESI) *m/z* calcd for $C_{25}H_{21}BrNO_3S$ [M+H$^+$]: 499.0420, found 499.0421.

5-(((4-Iodophenyl)sulfonyl)methyl)-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3aj)



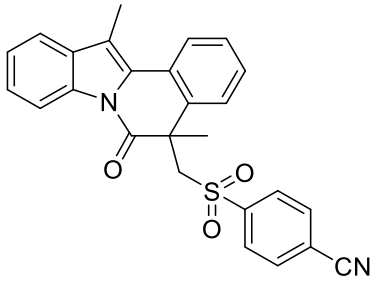
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3aj** (76%, yellow solid). mp 233-235 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.39 (m, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.53 – 7.51 (m, 1H), 7.45 (d, *J* = 8.1 Hz, 2H), 7.36 – 7.27 (m, 3H), 7.17 – 7.05 (m, 4H), 4.48 (d, *J* = 14.7 Hz, 1H), 3.86 (d, *J* = 14.7 Hz, 1H), 2.59 (s, 3H), 1.54 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.9, 139.4, 138.0, 134.2, 134.1, 132.4, 129.2, 129.1, 127.9, 127.6, 127.2, 126.3, 126.1, 125.2, 124.6, 118.6, 116.9, 115.4, 101.6, 64.5, 46.4, 31.8, 11.8. HRMS (ESI) *m/z* calcd for $C_{25}H_{21}INO_3S$ [M+H$^+$]: 542.0281, found 542.0280.

5,12-Dimethyl-5-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ak)



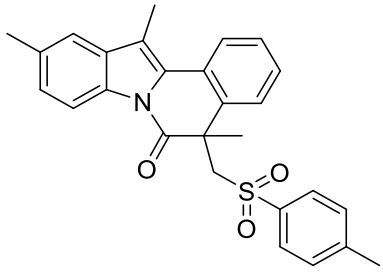
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ak** (72%, white solid). mp 209-211 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 – 8.49 (m, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.63 – 7.59 (m, 3H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.43 – 7.36 (m, 3H), 7.22 – 7.11 (m, 2H), 4.62 (d, *J* = 14.6 Hz, 1H), 4.00 (d, *J* = 14.7 Hz, 1H), 2.68 (s, 3H), 1.64 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.8, 143.4, 134.8 (q, J_{C-F} = 32.7 Hz), 134.2, 134.0, 132.4, 129.0, 128.4, 128.0, 127.5, 127.0, 126.4, 126.1, 125.9 (q, J_{C-F} = 3.6 Hz), 125.2, 124.6, 123.0 (q, J_{C-F} = 271.6 Hz), 118.6, 116.8, 115.5, 64.4, 46.5, 31.6, 11.7. HRMS (ESI) *m/z* calcd for $C_{26}H_{21}F_3NO_3S$ [M+H$^+$]: 484.1189, found 484.1190.

4-(((5,12-Dimethyl-6-oxo-5,6-dihydroindolo[2,1-*a*]isoquinolin-5-yl)methyl)sulfonyl)benzonitrile (3al)



Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3al** (70%, yellow solid). mp 221-223 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 – 8.44 (m, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.62 – 7.55 (m, 3H), 7.47 – 7.37 (m, 5H), 7.23 – 7.15 (m, 2H), 4.59 (d, *J* = 14.8 Hz, 1H), 3.99 (d, *J* = 14.8 Hz, 1H), 2.67 (s, 3H), 1.63 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 143.9, 134.1, 133.9, 132.4, 132.4, 129.0, 128.4, 128.1, 127.6, 127.1, 126.3, 126.2, 125.3, 124.9, 118.7, 117.1, 116.8, 116.7, 115.6, 64.4, 46.5, 31.6, 11.7. HRMS (ESI) *m/z* calcd for $C_{26}H_{21}N_2O_3S$ [M+H$^+$]: 441.1267, found 441.1265.

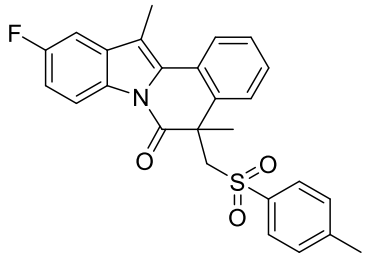
5,10,12-Trimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ba)



Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ba** (85%, yellow solid). mp 193-194 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.3 Hz, 1H),

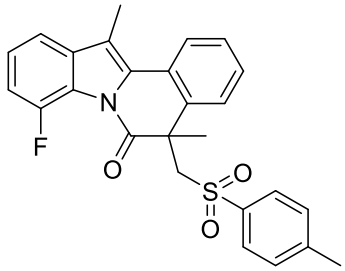
7.93 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.22 (m, 5H), 7.17 – 7.09 (m, 2H), 6.86 (d, *J* = 7.9 Hz, 2H), 4.47 (d, *J* = 14.6 Hz, 1H), 3.83 (d, *J* = 14.6 Hz, 1H), 2.55 (s, 3H), 2.41 (s, 3H), 2.05 (s, 3H), 1.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 144.4, 136.6, 134.3, 134.0, 132.6, 132.5, 129.4, 129.3, 127.9, 127.7, 127.4, 127.0, 126.3, 125.0, 118.4, 116.6, 114.8, 64.4, 46.3, 31.9, 21.7, 21.4, 11.7. HRMS (ESI) *m/z* calcd for $C_{27}H_{26}NO_3S$ [M+H$^+$]: 444.1628, found 444.1630.

10-Fluoro-5,12-dimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ca)



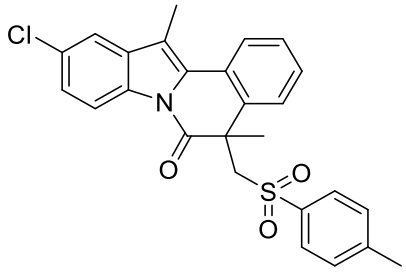
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ca** (67%, yellow oil). mp 179-181 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (dd, *J* = 8.9, 4.8 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.34 – 7.30 (m, 1H), 7.28 – 7.22 (m, 3H), 7.18 – 7.13 (m, 2H), 7.02 – 6.97 (m, 1H), 6.91 (d, *J* = 8.0 Hz, 2H), 4.46 (d, *J* = 14.6 Hz, 1H), 3.85 (d, *J* = 14.6 Hz, 1H), 2.55 (s, 3H), 2.12 (s, 3H), 1.54 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 160.4 (d, J_{C-F} = 242.1 Hz), 144.5, 136.7, 134.5, 133.9 (d, J_{C-F} = 9.4 Hz), 130.9, 130.5, 129.4, 127.9, 127.4, 125.9, 125.2, 118.1, 118.0, 114.4 (d, J_{C-F} = 4.1 Hz), 113.2, 113.0, 104.3 (d, J_{C-F} = 24.1 Hz), 64.5, 46.3, 31.8, 21.4, 11.8. HRMS (ESI) *m/z* calcd for $C_{26}H_{23}FNO_3S$ [M+H$^+$]: 448.1377, found 448.1376.

8-Fluoro-5,12-dimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3da)



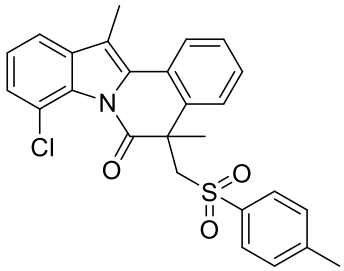
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3da** (74%, yellow solid). mp 163-164 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.14 (m, 7H), 7.02 – 6.93 (m, 3H), 4.46 (d, *J* = 14.5 Hz, 1H), 3.82 (d, *J* = 14.5 Hz, 1H), 2.55 (s, 3H), 2.11 (s, 3H), 1.58 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 151.8, 149.2, 144.4, 137.0, 136.8 (d, J_{C-F} = 3.9 Hz), 134.9, 131.8, 129.4, 128.0, 127.8, 127.4, 126.2, 125.5, 125.4, 121.1 (d, J_{C-F} = 11.3 Hz), 115.2, 114.5 (d, J_{C-F} = 3.5 Hz), 113.3 (d, J_{C-F} = 23.2 Hz), 64.7, 47.0, 31.6, 21.5, 11.9. HRMS (ESI) *m/z* calcd for $C_{26}H_{23}FNO_3S$ [M+H$^+$]: 448.1377, found 448.1379.

10-Chloro-5,12-dimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ea)



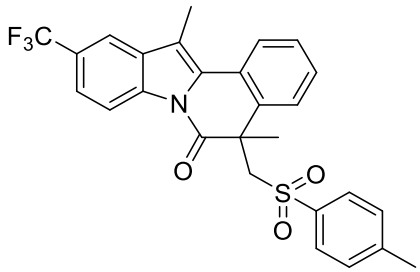
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ea** (60%, white solid). mp 201-203 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.6 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 2.0 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.20 (m, 4H), 7.17 – 7.11 (m, 1H), 6.90 (d, *J* = 8.0 Hz, 2H), 4.44 (d, *J* = 14.6 Hz, 1H), 3.85 (d, *J* = 14.6 Hz, 1H), 2.53 (s, 3H), 2.10 (s, 3H), 1.53 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 144.5, 136.7, 134.5, 133.9, 132.6, 130.7, 130.1, 129.4, 127.9, 127.9, 127.8, 127.4, 125.8, 125.6, 125.3, 118.2, 118.0, 114.1, 64.5, 46.4, 31.8, 21.4, 11.7. HRMS (ESI) *m/z* calcd for $C_{26}H_{23}ClNO_3S$ [M+H$^+$]: 464.1082, found 464.1084.

8-Chloro-5,12-dimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3fa)



Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3fa** (65%, yellow solid). mp 189-190 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.41 – 7.39 (m, 1H), 7.35 – 7.23 (m, 5H), 7.21 – 7.16 (m, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 4.46 (d, *J* = 14.4 Hz, 1H), 3.78 (d, *J* = 14.4 Hz, 1H), 2.55 (s, 3H), 2.20 (s, 3H), 1.66 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.3, 144.2, 137.6, 136.9, 135.3, 133.3, 132.8, 129.5, 128.0, 127.9, 127.7, 127.5, 127.4, 127.0, 125.5, 125.5, 122.6, 117.4, 114.7, 64.3, 47.4, 30.9, 21.5, 11.6. HRMS (ESI) *m/z* calcd for $C_{26}H_{23}ClNO_3S$ [M+H$^+$]: 464.1082, found 464.1083.

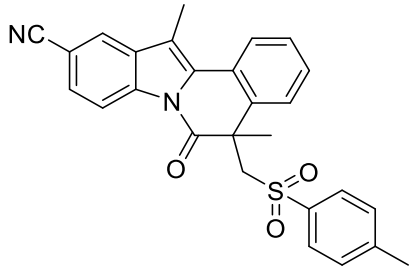
5,12-Dimethyl-5-(tosylmethyl)-10-(trifluoromethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ga)



Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ga** (58%, white solid). mp 212-214 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.6 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.78 (s, 1H), 7.55 – 7.52 (m, 1H), 7.37 – 7.15 (m, 5H), 6.92 (d, *J* = 8.0 Hz, 2H), 4.46 (d, *J* = 14.6 Hz, 1H), 3.87 (d, *J* = 14.6 Hz, 1H), 2.62 (s, 3H), 2.10 (s, 3H), 1.56 (s,

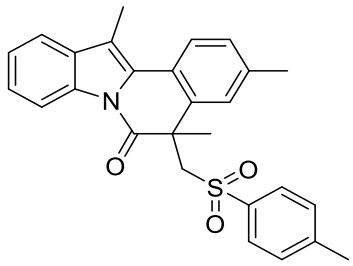
3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.5, 144.5, 136.8, 135.8, 134.5, 132.3, 131.1, 129.4, 128.1 128.0, 127.8, 127.4, 126.6 (q, J_{C-F} = 32.0 Hz), 125.7, 125.4, 124.7(q, J_{C-F} = 270.4 Hz), 122.3 (q, J_{C-F} = 3.5 Hz), 117.1, 115.7 (q, J_{C-F} = 4.1 Hz), 114.5, 64.6, 46.5, 31.7, 21.4, 11.6. HRMS (ESI) *m/z* calcd for $C_{27}H_{23}F_3NO_3S$ [M+H$^+$]: 498.1345, found 498.1343.

5,12-Dimethyl-6-oxo-5-(tosylmethyl)-5,6-dihydroindolo[2,1-*a*]isoquinoline-10-carbonitrile (3ha)



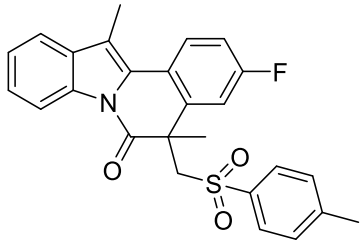
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ha** (63%, yellow solid). mp 207-209 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.83 (s, 1H), 7.54 (d, *J* = 6.9 Hz, 1H), 7.36 – 7.28 (m, 3H), 7.23 – 7.16 (m, 2H), 6.97 (d, *J* = 7.8 Hz, 2H), 4.45 (d, *J* = 14.6 Hz, 1H), 3.90 (d, *J* = 14.6 Hz, 1H), 2.59 (s, 3H), 2.17 (s, 3H), 1.56 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.8, 144.5, 137.0, 136.1, 134.5, 132.6, 131.6, 129.5, 128.7, 128.4, 128.1, 127.7, 127.4, 125.6, 125.4, 123.1, 119.7, 117.6, 114.0, 107.6, 64.6, 46.7, 31.6, 21.5, 11.6. HRMS (ESI) *m/z* calcd for $C_{27}H_{23}N_2O_3S$ [M+H$^+$]: 455.1424, found 455.1425.

3,5,12-Trimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ia)[4]



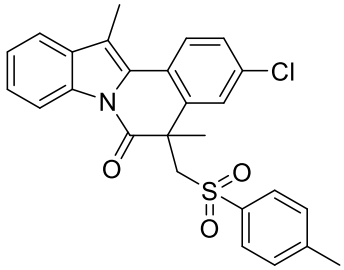
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ia** (60%, yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 – 8.36 (m, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.52 – 7.50 (m, 1H), 7.34 – 7.23 (m, 6H), 7.17 – 7.13 (m, 1H), 6.88 (d, *J* = 8.0 Hz, 2H), 4.48 (d, *J* = 14.6 Hz, 1H), 3.85 (d, *J* = 14.6 Hz, 1H), 2.59 (s, 3H), 2.06 (s, 3H), 1.54 (s, 3H).

3-Fluoro-5,12-dimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ja)[4]



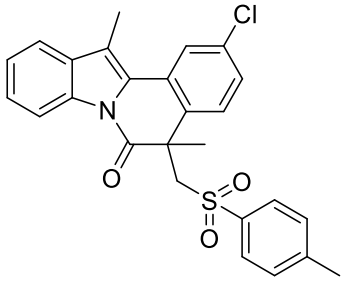
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ja** (58%, yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 – 8.45 (m, 1H), 8.01 (dd, *J* = 9.0, 5.6 Hz, 1H), 7.60 – 7.57 (m, 1H), 7.40 – 7.34 (m, 4H), 7.12 – 7.07 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.96 – 6.93 (m, 1H), 4.55 (d, *J* = 14.7 Hz, 1H), 3.85 (d, *J* = 14.7 Hz, 1H), 2.64 (s, 3H), 2.20 (s, 3H), 1.61 (s, 3H).

3-Chloro-5,12-dimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ka)[4]



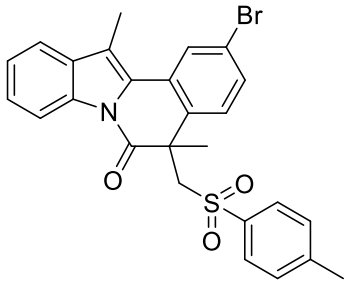
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ka** (71%, yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 7.0 Hz, 1H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.42 – 7.26 (m, 5H), 7.08 (d, *J* = 2.1 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 2H), 4.57 (d, *J* = 14.8 Hz, 1H), 3.87 (d, *J* = 14.8 Hz, 1H), 2.64 (s, 3H), 2.24 (s, 3H), 1.61 (s, 3H).

2-Chloro-5,12-dimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3la)



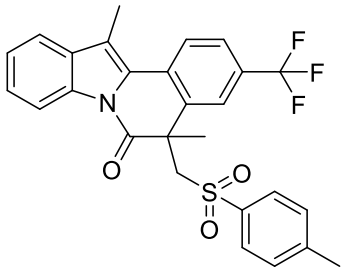
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3la** (63%, yellow solid). mp 188-189 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 – 8.48 (m, 1H), 7.98 (d, *J* = 2.0 Hz, 1H), 7.62 – 7.60 (m, 1H), 7.43 – 7.34 (m, 4H), 7.20 – 7.17 (m, 1H), 7.11 – 7.09 (m, 1H), 7.02 – 6.95 (m, 2H), 4.55 (d, *J* = 14.7 Hz, 1H), 3.88 (d, *J* = 14.7 Hz, 1H), 2.68 (s, 3H), 2.20 (s, 3H), 1.60 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.5, 144.7, 136.6, 134.4, 133.9, 132.6, 132.1, 129.4, 128.9, 128.0, 127.8, 127.8, 127.4, 126.3, 124.6, 124.6, 118.7, 117.0, 116.2, 64.4, 46.1, 31.6, 21.5, 11.7. HRMS (ESI) *m/z* calcd for $C_{26}H_{23}ClNO_3S$ [M+H$^+$]: 464.1082, found 464.1081.

2-Bromo-5,12-dimethyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ma)



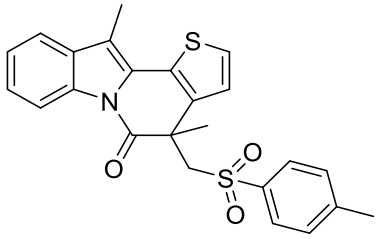
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3ma** (62%, yellow solid). mp 198-200 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 7.8 Hz, 1H), 8.05 (s, 1H), 7.54 (d, *J* = 7.4 Hz, 1H), 7.35 – 7.26 (m, 4H), 7.18 – 7.14 (m, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.94 (d, *J* = 7.8Hz, 2H), 4.47 (d, *J* = 14.6 Hz, 1H), 3.80 (d, *J* = 14.6 Hz, 1H), 2.60 (s, 3H), 2.14 (s, 3H), 1.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.5, 144.7, 136.6, 134.4, 133.1, 132.1, 130.2, 129.5, 129.1, 128.2, 127.9, 127.8, 127.5, 126.3, 124.6, 122.0, 118.7, 117.0, 116.2, 64.3, 46.2, 31.6, 21.5, 11.7. HRMS (ESI) *m/z* calcd for $C_{26}H_{23}BrNO_3S$ [M+H$^+$]: 508.0577, found 508.0578.

5,12-Dimethyl-5-(tosylmethyl)-3-(trifluoromethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3na)[4]



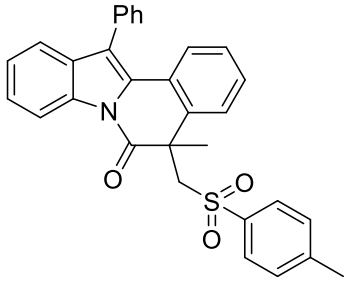
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3na** (62%, yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 8.0 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.65 – 7.57 (m, 2H), 7.45 – 7.37 (m, 3H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 4.61 (d, *J* = 14.8 Hz, 1H), 3.95 (d, *J* = 14.8 Hz, 1H), 2.71 (s, 3H), 2.23 (s, 3H), 1.65 (s, 3H).

4,11-Dimethyl-4-(tosylmethyl)thieno[2',3':3,4]pyrido[1,2-*a*]indol-5(4*H*)-one (3oa)



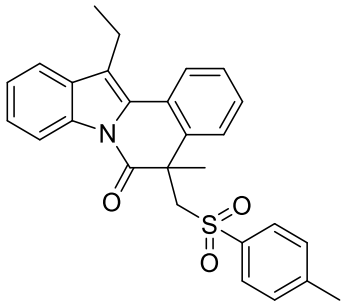
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3oa** (60%, yellow oil). mp 152-154 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.25 (m, 1H), 7.44 – 7.41 (m, 1H), 7.28 – 7.18 (m, 5H), 6.84 – 6.80 (m, 3H), 4.38 (d, *J* = 14.5 Hz, 1H), 3.66 (d, *J* = 14.5 Hz, 1H), 2.41 (s, 3H), 1.96 (s, 3H), 1.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 144.7, 136.1, 135.6, 134.5, 131.7, 129.2, 128.0, 127.6, 126.1, 126.1, 125.6, 125.5, 124.5, 118.4, 116.4, 112.8, 64.6, 45.6, 30.7, 21.3, 9.7. HRMS (ESI) *m/z* calcd for $C_{24}H_{22}NO_3S_2$ [M+H$^+$]: 436.1036, found 436.1038.

5-Methyl-12-phenyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3pa)[4]



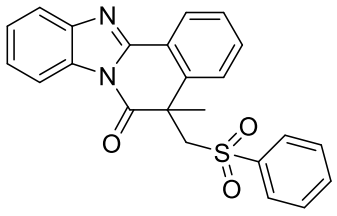
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3pa** (64%, yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 8.2 Hz, 1H), 7.52 – 7.28 (m, 9H), 7.20 – 7.17 (m, 3H), 7.08 – 7.04 (m, 1H), 6.96 – 6.90 (m, 3H), 4.51 (d, *J* = 14.6 Hz, 1H), 3.87 (d, *J* = 14.6 Hz, 1H), 2.04 (s, 3H), 1.59 (s, 3H).

12-Ethyl-5-methyl-5-(tosylmethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3qa)



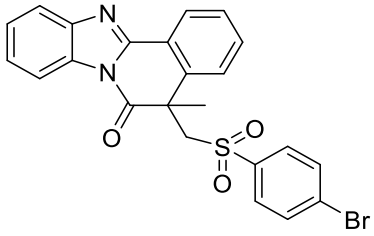
Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **3qa** (68%, yellow solid). mp 173-174 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 – 8.35 (m, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.51 – 7.49 (m, 1H), 7.34 – 7.24 (m, 6H), 7.18 – 7.14 (m, 1H), 6.85 (d, *J* = 7.9 Hz, 2H), 4.48 (d, *J* = 14.6 Hz, 1H), 3.84 (d, *J* = 14.6 Hz, 1H), 3.07 (q, *J* = 7.6 Hz, 2H), 2.00 (s, 3H), 1.52 (s, 3H), 1.35 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 144.5, 136.4, 134.4, 134.3, 131.6, 129.3, 128.6, 128.0, 127.6, 127.6, 125.9, 125.8, 124.7, 124.4, 121.6, 118.2, 117.1, 64.3, 46.4, 32.0, 21.3, 18.7, 13.4. HRMS (ESI) *m/z* calcd for $C_{27}H_{26}NO_3S$ [M+H$^+$]: 444.1628, found 444.1626.

5-Methyl-5-((phenylsulfonyl)methyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (5ab)[5]



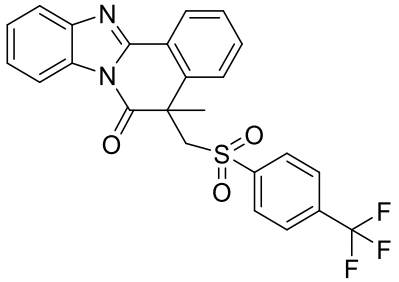
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **5ab** (64%, white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 7.8 Hz, 1H), 8.27 – 8.25 (m, 1H), 7.78 – 7.76 (m, 1H), 7.41 – 7.30 (m, 6H), 7.21 – 7.17 (m, 3H), 7.10 (d, *J* = 7.9 Hz, 1H), 4.48 (d, *J* = 14.8 Hz, 1H), 3.96 (d, *J* = 14.8 Hz, 1H), 1.60 (s, 3H).

5-(((4-Bromophenyl)sulfonyl)methyl)-5-methylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (5ai)[5]



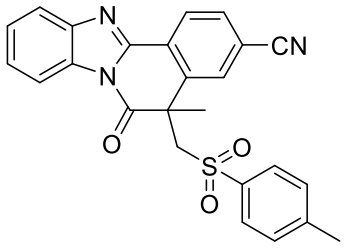
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **5ai** (55%, yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 7.9 Hz, 1H), 8.24 – 8.22 (m, 1H), 7.78 – 7.76 (m, 1H), 7.42 – 7.30 (m, 5H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.20 – 7.18 (m, 2H), 7.11 (d, *J* = 7.9 Hz, 1H), 4.47 (d, *J* = 14.8 Hz, 1H), 3.94 (d, *J* = 14.8 Hz, 1H), 1.61 (s, 3H).

5-Methyl-5-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (5ak)[6]



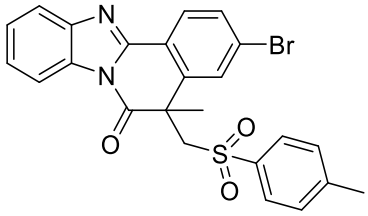
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **5ak** (48%, yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 7.8 Hz, 1H), 8.25 – 8.23 (m, 1H), 7.78 – 7.76 (m, 1H), 7.50 – 7.34 (m, 7H), 7.19 – 7.13 (m, 1H), 7.05 (d, *J* = 7.9 Hz, 1H), 4.51 (d, *J* = 14.9 Hz, 1H), 3.98 (d, *J* = 14.9 Hz, 1H), 1.63 (s, 3H).

5-Methyl-6-oxo-5-(tosylmethyl)-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-3-carbonitrile (5ba)[3]



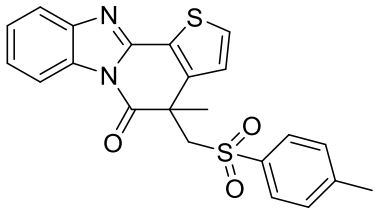
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **5ba** (80%, yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.2 Hz, 1H), 8.26 – 8.24 (m, 1H), 7.80 – 7.77 (m, 1H), 7.60 (d, *J* = 8.1 Hz, 1H), 7.43 – 7.40 (m, 2H), 7.33 (s, 1H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 4.49 (d, *J* = 15.0 Hz, 1H), 3.94 (d, *J* = 15.1 Hz, 1H), 2.23 (s, 3H), 1.61 (s, 3H).

3-Bromo-5-methyl-5-(tosylmethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (5ca)[3]



Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **5ca** (68%, yellow solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.23 (m, 2H), 7.76 – 7.74 (m, 1H), 7.46 – 7.37 (m, 3H), 7.19 (d, *J* = 1.8 Hz, 2H), 7.09 (s, 1H), 6.97 (d, *J* = 8.0 Hz, 2H), 4.47 (d, *J* = 15.0 Hz, 1H), 3.87 (d, *J* = 15.0 Hz, 1H), 2.20 (s, 3H), 1.59 (s, 3H).

4-Methyl-4-(tosylmethyl)benzo[4,5]imidazo[1,2-*a*]thieno[2,3-c]pyridin-5(4*H*)-one (5da)[3]

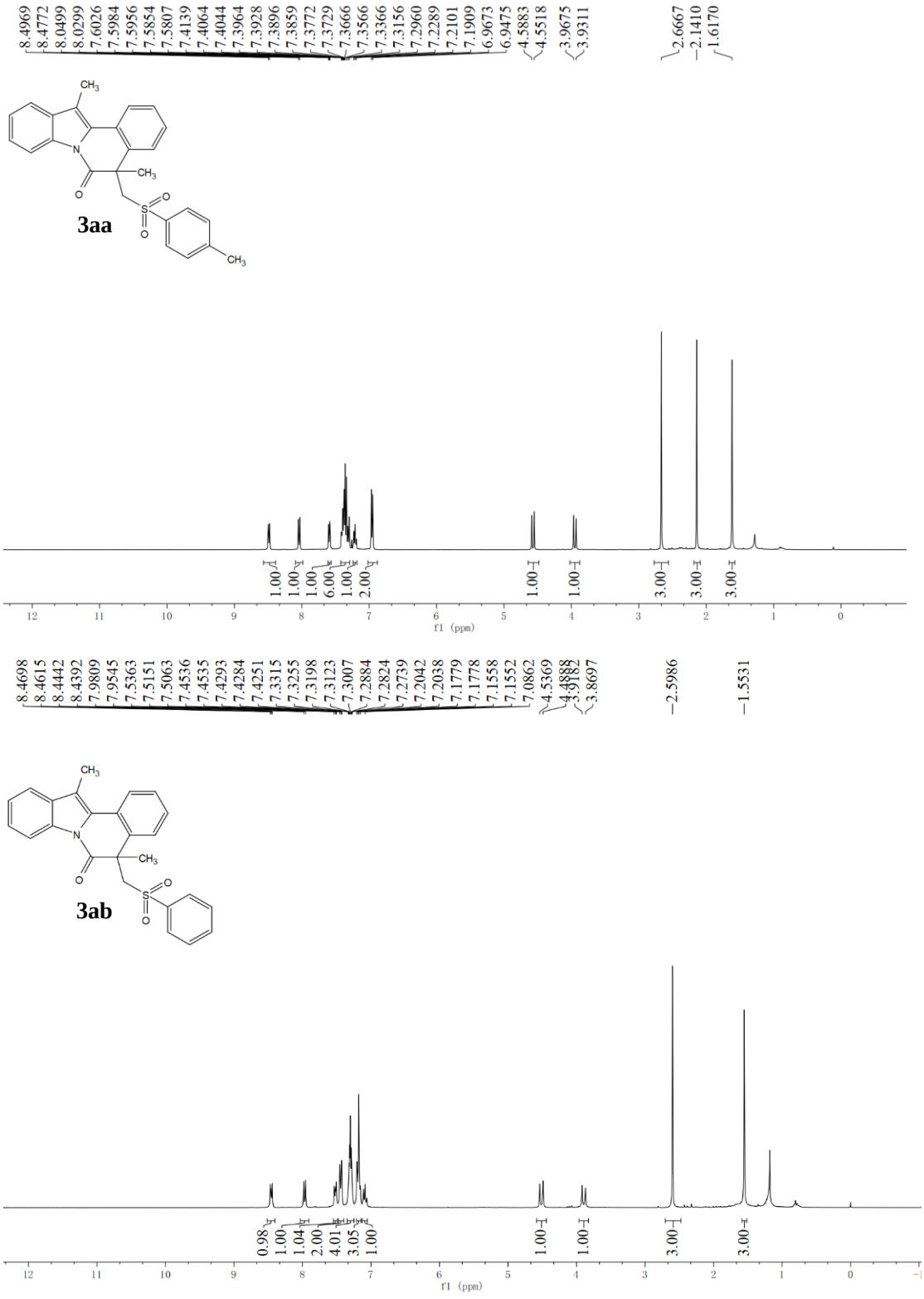


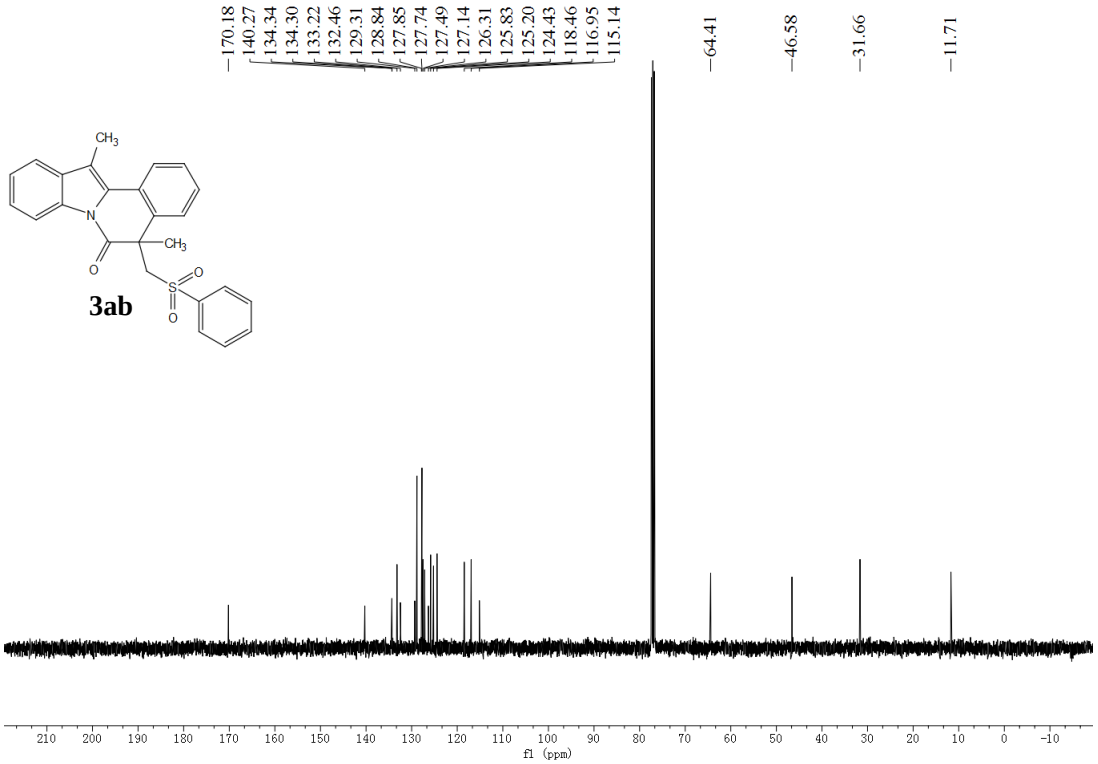
Known compound. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate 3:1) gave **5da** (40%, white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 – 8.08 (m, 1H), 7.70 – 7.68 (m, 1H), 7.36 – 7.32 (m, 3H), 7.25 – 7.19 (m, 2H), 6.92 (d, *J* = 7.9 Hz, 2H), 6.82 (d, *J* = 5.0 Hz, 1H), 4.37 (d, *J* = 14.6 Hz, 1H), 3.76 (d, *J* = 14.6 Hz, 1H), 2.02 (s, 3H), 1.56 (s, 3H).

5. References

1. Y.-L. Wei, J.-Q. Chen, B. Sun and P.-F. Xu, *Chem. Commun.*, 2019, **55**, 5922.
2. X. Ma and S. B. Herzon, *Beilstein J. Org. Chem.*, 2019, **14**, 2259.
3. Y. Tang, M. Yang, F. Wang, X. Hu and G. Wang, *Tetrahedron Lett.*, 2019, **67**, 152845.
4. Z.-J. Shen, B. Huang, N. Ma, L. Yao, C. Yang, L. Guo and W. Xia, *Adv. Synth. Catal.*, 2019, **363**, 1944.
5. Q. Liu, L. Wang, J. Liu, S. Ruan and P. Li, *Org. Biomol. Chem.*, 2019, **19**, 3489.
6. C. Wang, G. Sun, H.-L. Huang, J. Liu, H. Tang, Y. Li, H. Hu, S. He and F. Gao, *Chem. Asian J.*, 2019, **16**, 2618.

6. Copies of the ^{1}H NMR and ^{13}C NMR Spectra

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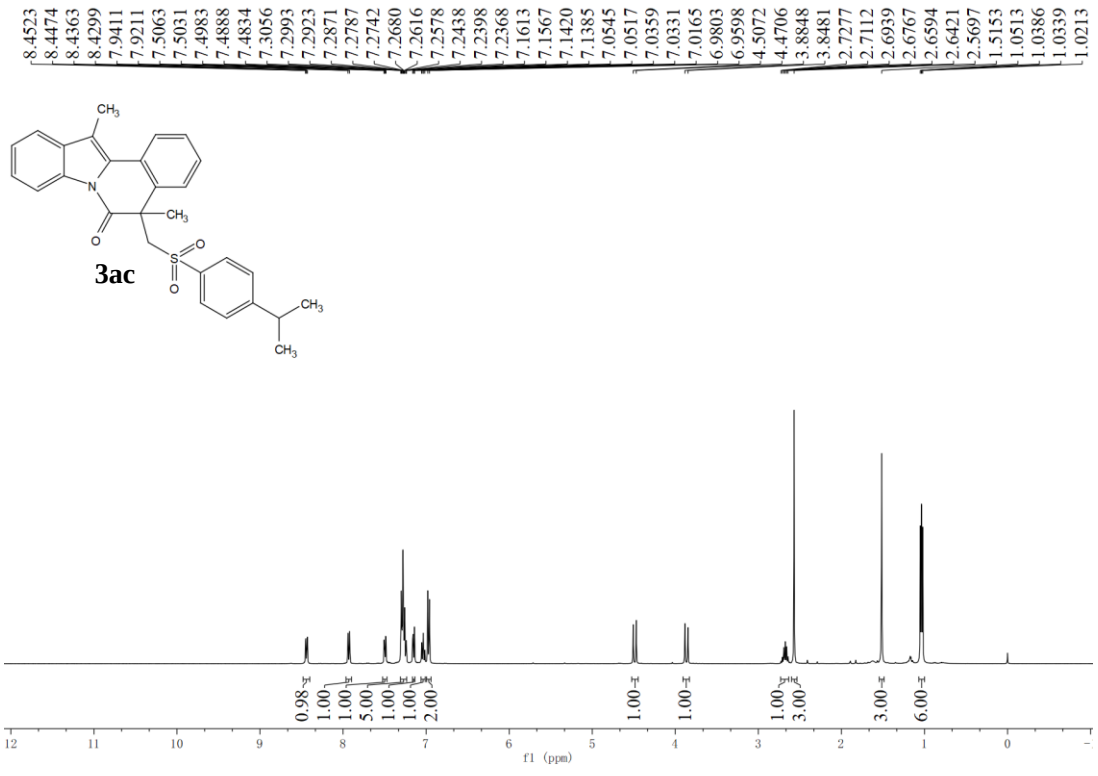
134.34
134.30
133.22
132.46
129.31
128.84
127.85
127.74
127.49
127.14
126.31
125.83
125.20
124.43
118.46
116.95
115.14
64.41
46.58
31.66
11.71
CH3
CH3
O
S
O
O
3ab
f1 (ppm)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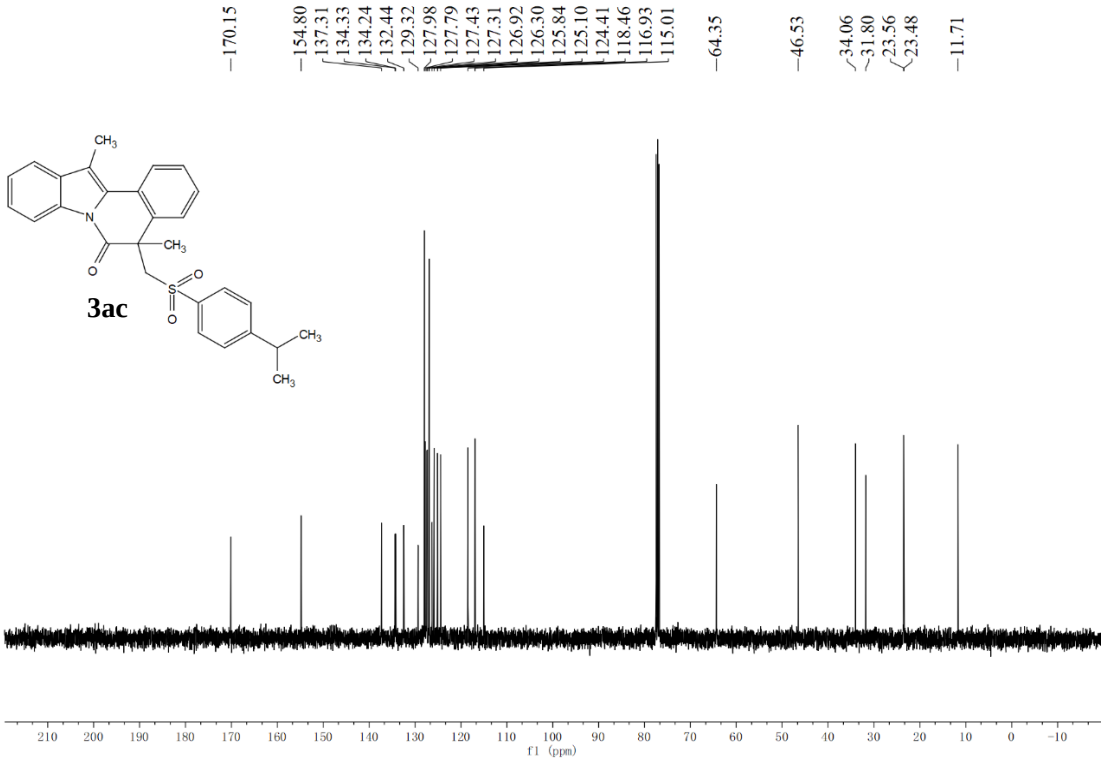
7.4834
7.3056
7.2993
7.2923
7.2871
7.2787
7.2742
7.2680
7.2616
7.2578
7.2438
7.2398
7.2368
7.1613
7.1567
7.1420
7.1385
7.0545
7.0517
7.0359
7.0331
7.0165
6.9803
6.9598
4.5072
4.4706
3.8848
3.8481
2.7277
2.7112
2.6939
2.6767
2.6594
2.6421
2.5697
1.5153
1.0513
1.0386
1.0339
1.0213
CH3
CH3
O
S
O
O
CH3
CH3
3ac
0.98
1.00
1.00
5.00
1.00
1.00
2.00
1.00
1.00
1.00
3.00
3.00
6.00
f1 (ppm)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127.98
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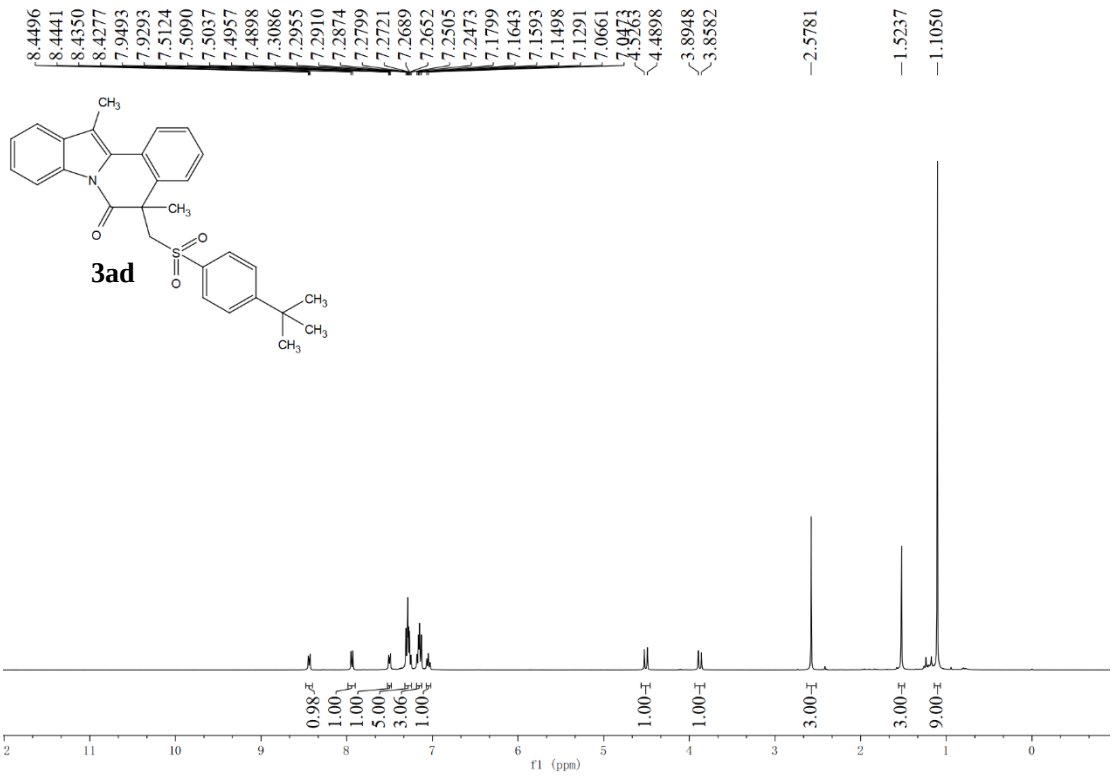
127.43
127.31
126.92
126.30
125.84
125.10
124.41
118.46
116.93
115.01
64.35
46.53
34.06
31.80
23.56
23.48
11.71
3ac
f1 (ppm)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7.4898
7.3086
7.2955
7.2910
7.2874
7.2799
7.2721
7.2689
7.2652
7.2505
7.2473
7.1799
7.1643
7.1593
7.1498
7.1291
7.0661
4.5263
4.4898
3.8948
3.8582
2.5781
1.5237
1.1050
0.98
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1.00
1.00
3.00
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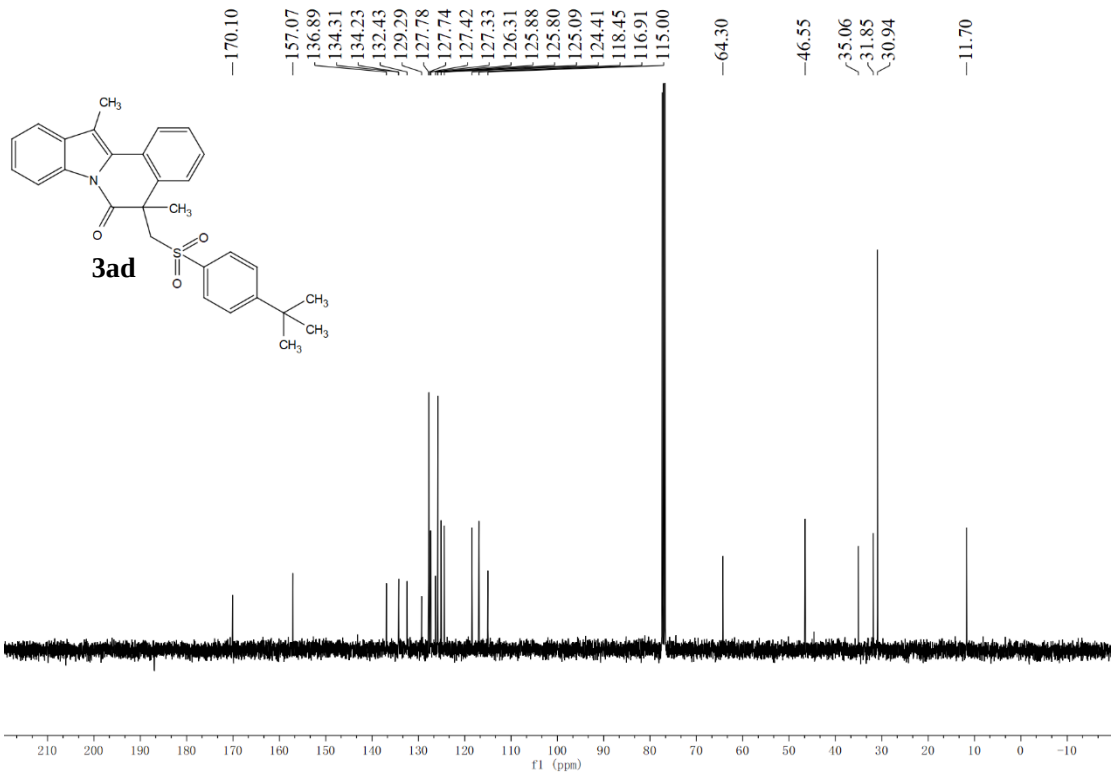
9.00
3ad
f1 (ppm)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127.42
127.33
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125.88
125.80
125.09
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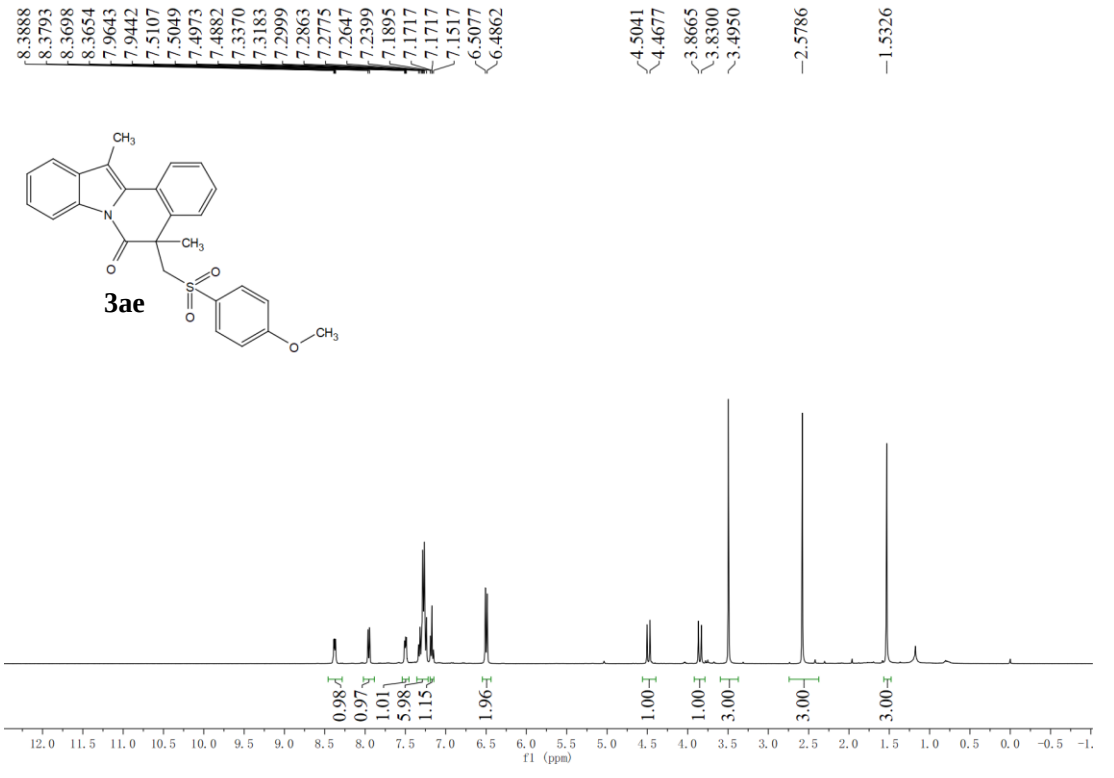
115.00
64.30
46.55
35.06
31.85
30.94
11.70
3ad
f1 (ppm)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7.3183
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7.1895
7.1717
7.1717
7.1517
6.5077
6.4862
4.5041
4.4677
3.8665
3.8300
3.4950
2.5786
1.5326
3ae
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5.98
1.15
1.96
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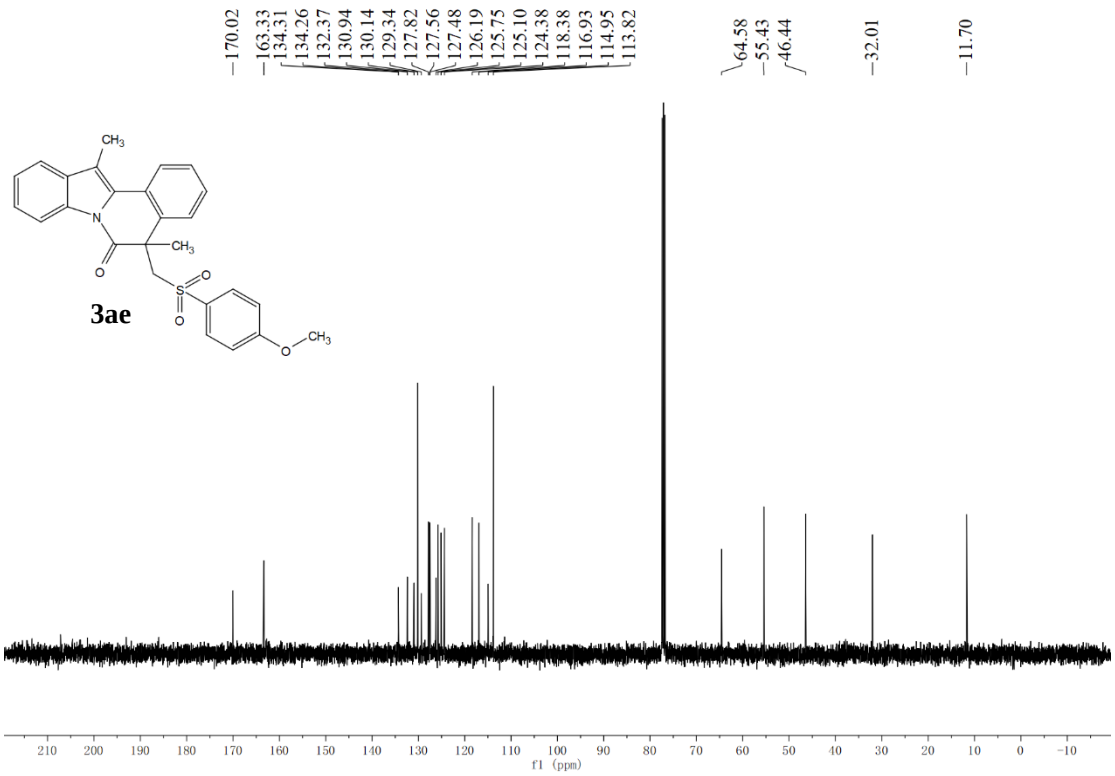
3.00
3.00
3.00
f1 (ppm)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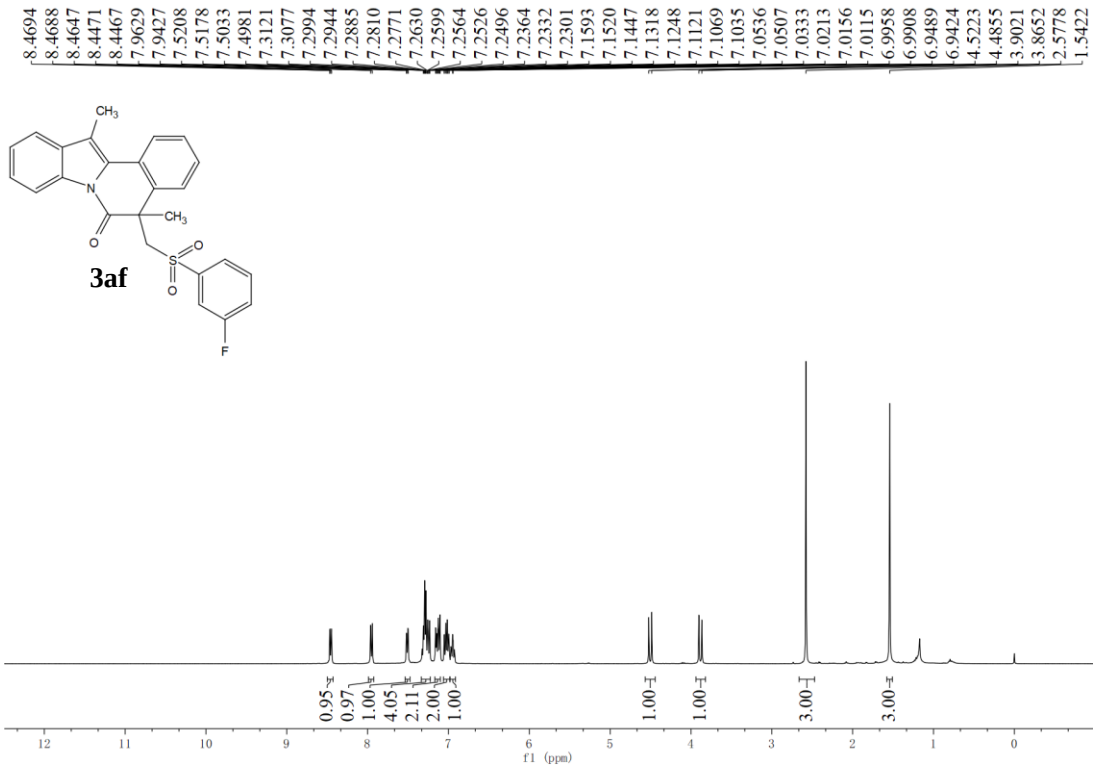
116.93
114.95
113.82
64.58
55.43
46.44
32.01
11.70
CH3
CH3
O
S
O
O
O
CH3
3ae
f1 (ppm)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7.0115
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6.9908
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6.9424
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1.5422
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CH3
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S
O
O
F
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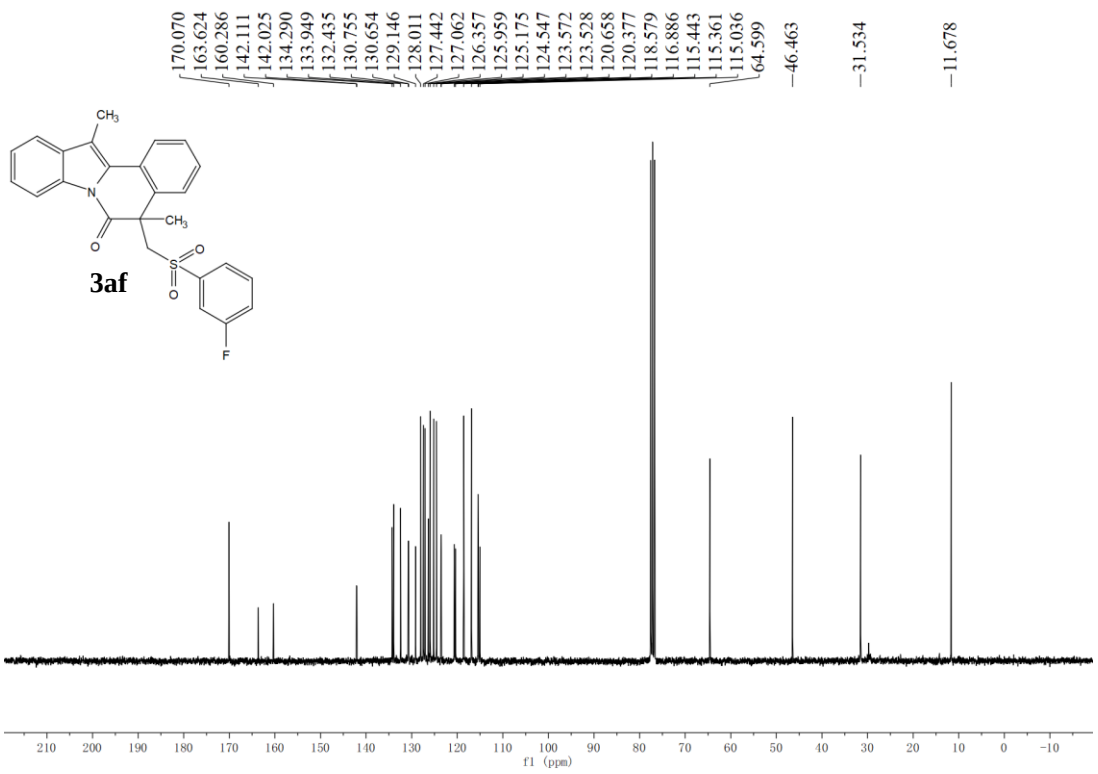
1.00
3.00
3.00
f1 (ppm)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125.175
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123.572
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115.361
115.036
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46.463
31.534
11.678
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S
O
O
F
3af
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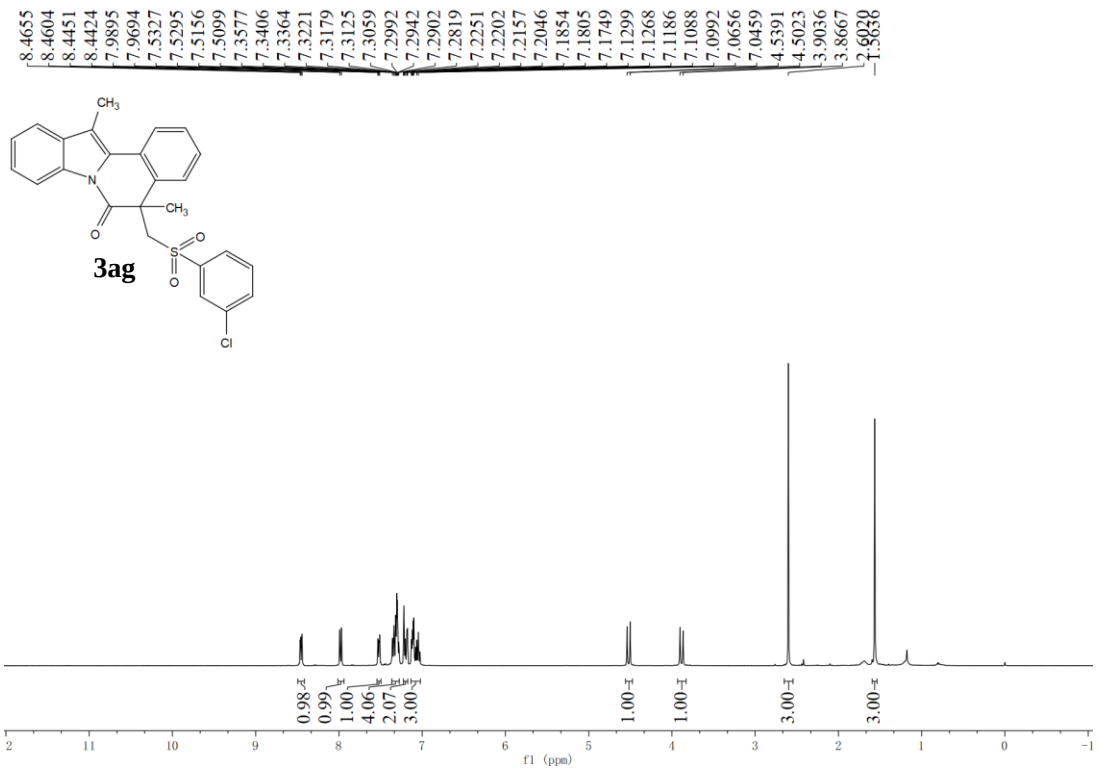
f1 (ppm)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7.2992
7.2942
7.2902
7.2819
7.2251
7.2202
7.2157
7.2046
7.1854
7.1805
7.1749
7.1299
7.1268
7.1186
7.1088
7.0992
7.0656
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3.8667
2.6020
1.5636
CH3
CH3
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N
S
O
O
Cl
3ag
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0.99
1.00
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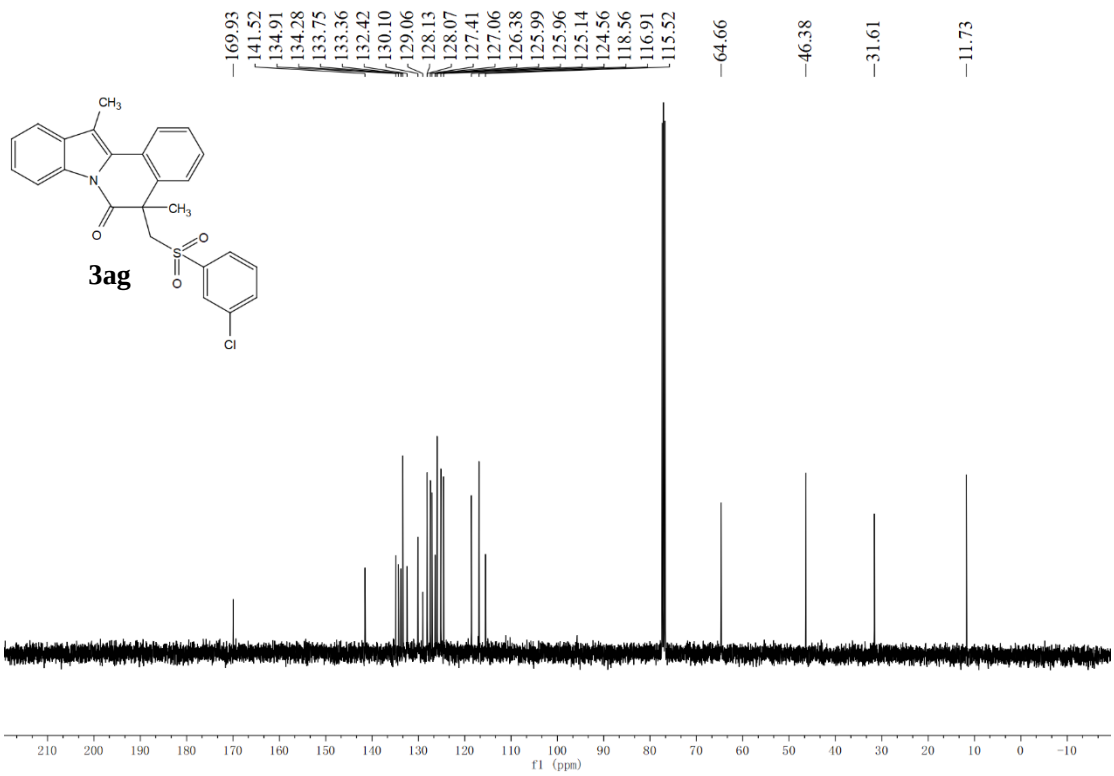
3.00
1.00
1.00
3.00
3.00
2 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)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125.96
125.14
124.56
118.56
116.91
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31.61
11.73
CH3
CH3
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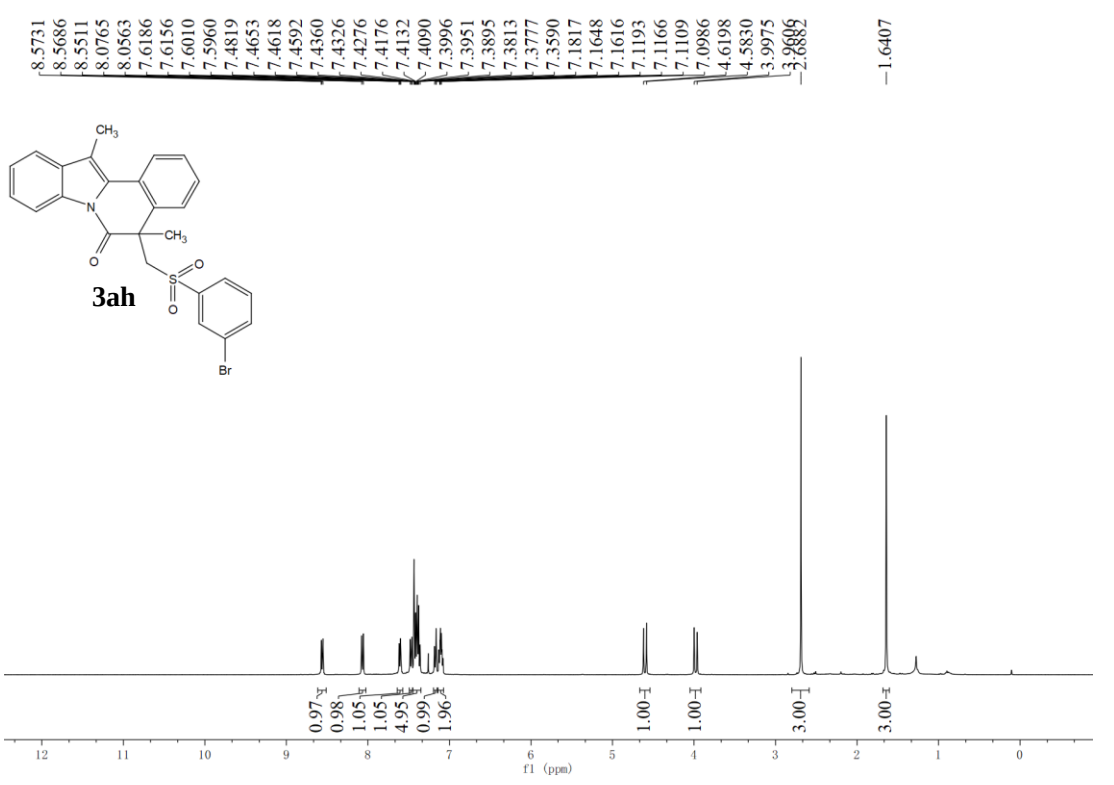
N
S
O
O
Cl
f1 (ppm)

3ag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CH3
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O
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Br
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0.99
1.96
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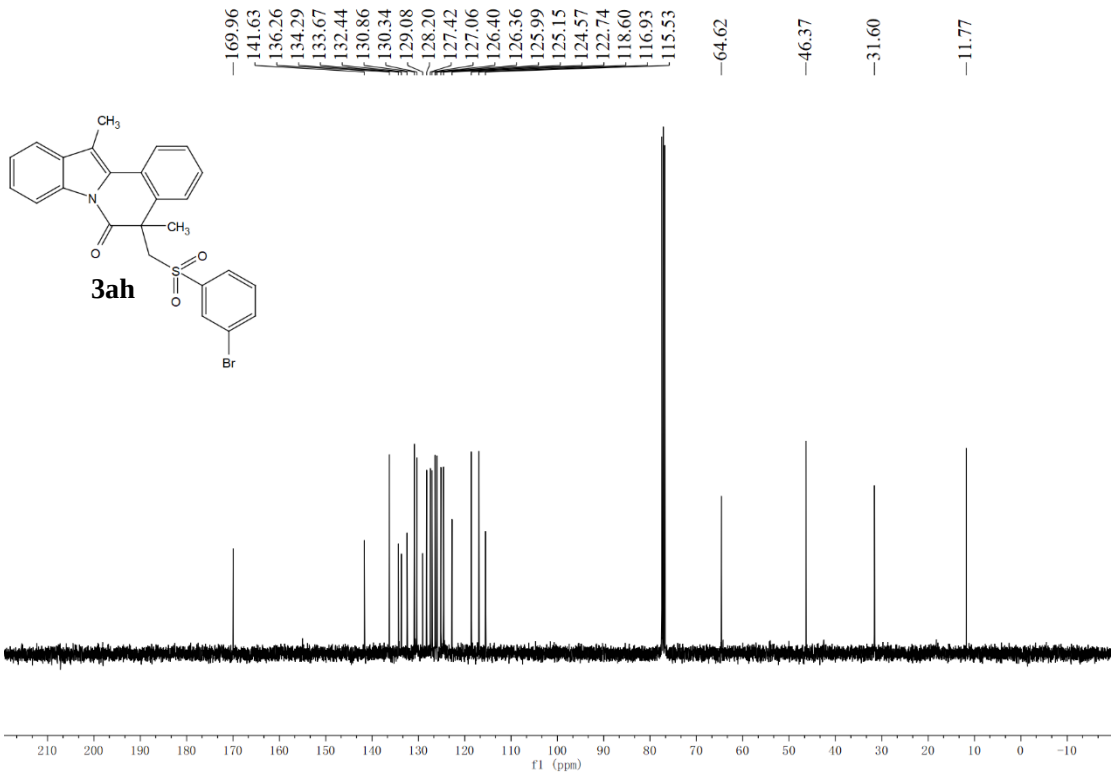
1.00
3.00
3.00
f1 (ppm)

3ah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124.57
122.74
118.60
116.93
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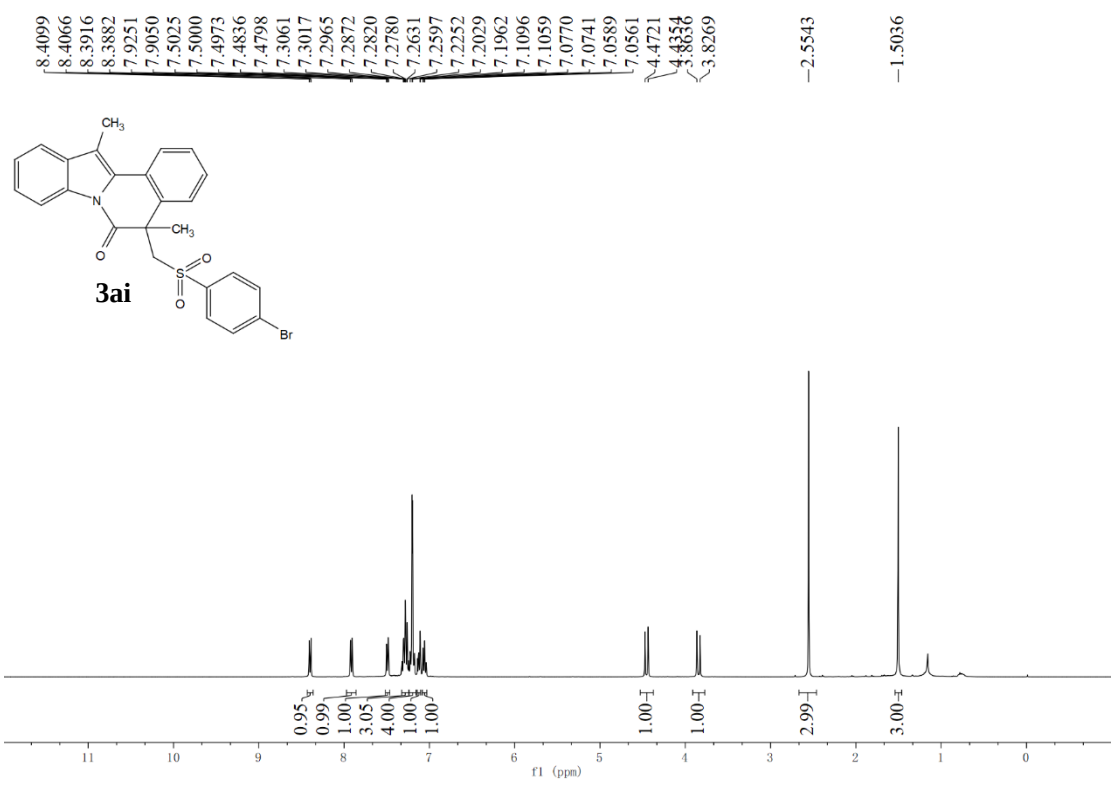
31.60
11.77
CH3
N
CH3
O
S
O
O
Br
f1 (ppm)

3ah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8.3916
8.3882
7.9251
7.9050
7.5025
7.5000
7.4973
7.4836
7.4798
7.3061
7.3017
7.2965
7.2872
7.2820
7.2780
7.2631
7.2597
7.2252
7.2029
7.1962
7.1096
7.1059
7.0770
7.0741
7.0589
7.0561
4.4721
4.4354
3.8636
3.8269
2.5543
1.5036
CH3
N
CH3
O
S
O
O
Br
0.95
0.99
1.00
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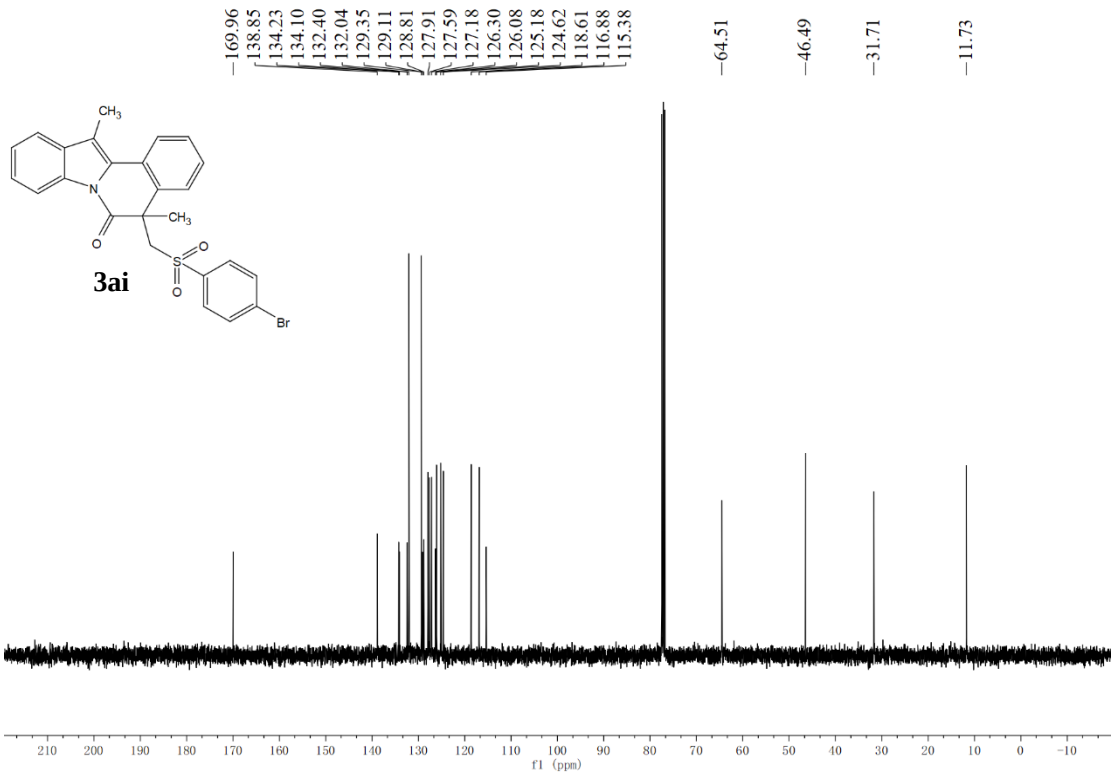
4.00
1.00
1.00
1.00
1.00
2.99
3.00
f1 (ppm)

3ai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129.11
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127.59
127.18
126.30
126.08
125.18
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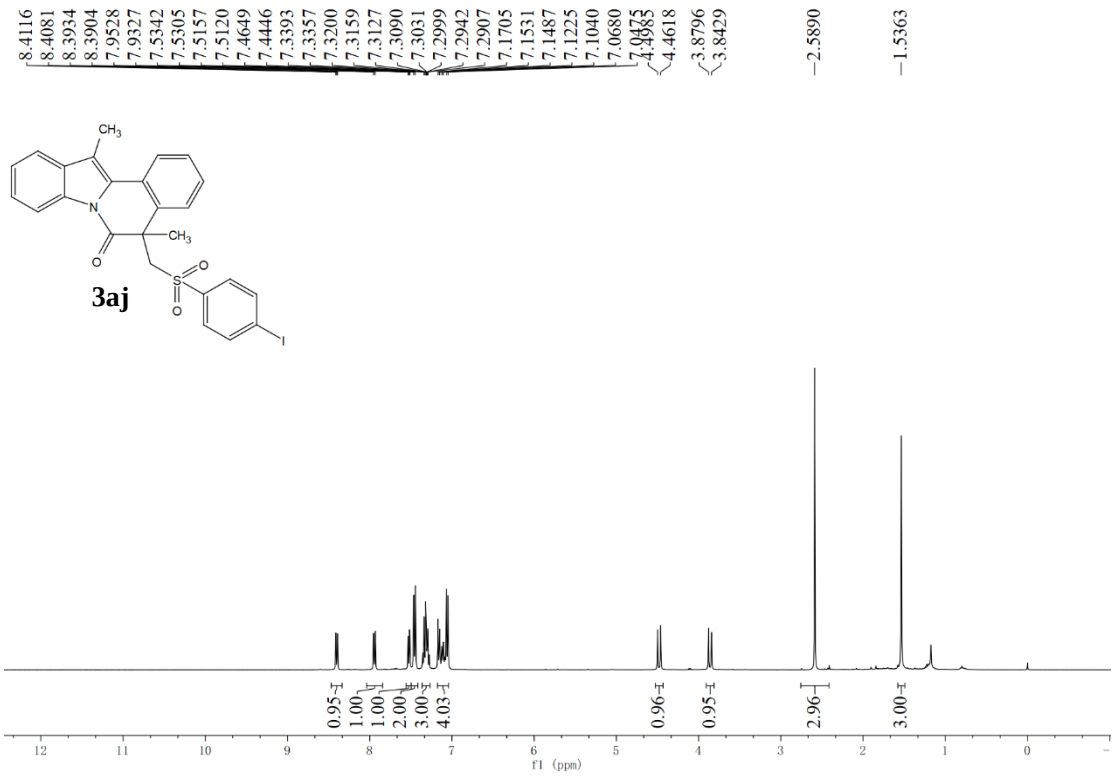
118.61
116.88
115.38
64.51
46.49
31.71
11.73
3ai
Br
f1 (ppm)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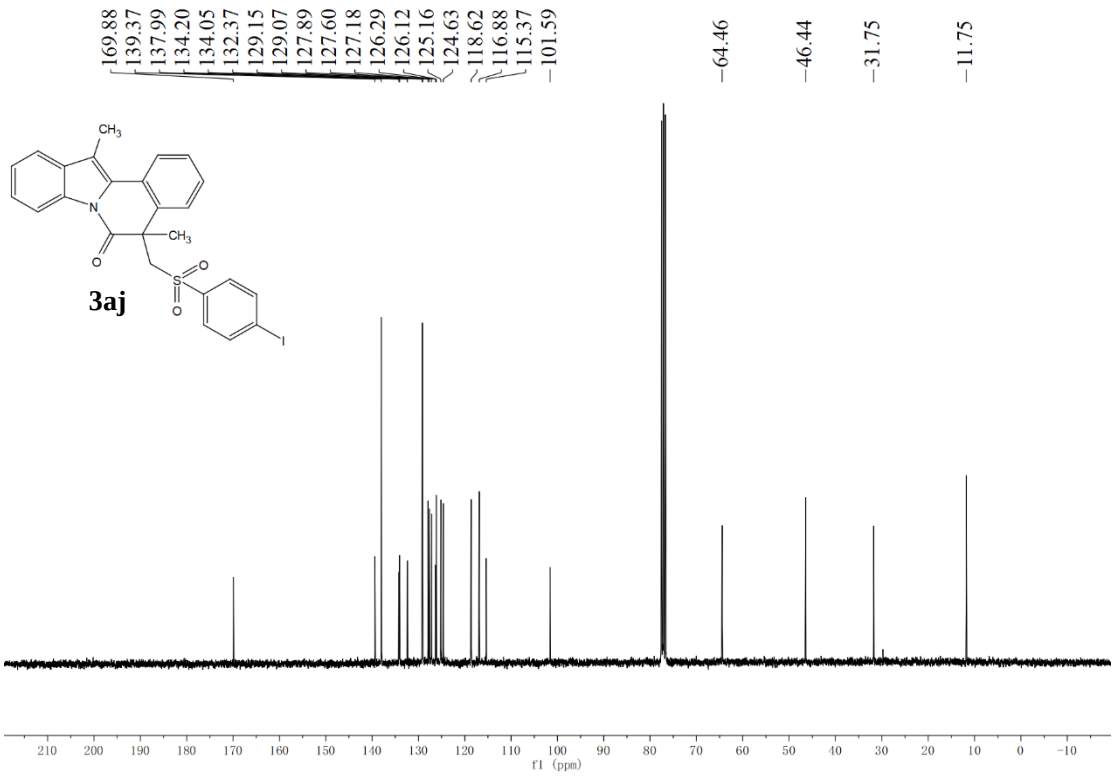
7.4446
7.3393
7.3357
7.3200
7.3159
7.3127
7.3090
7.3031
7.2999
7.2942
7.2907
7.1705
7.1531
7.1487
7.1225
7.1040
7.0680
4.4618
3.8796
3.8429
2.5890
1.5363
3aj
0.95
1.00
1.00
2.00
3.00
4.03
0.96
0.95
2.96
3.00
f1 (ppm)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129.07
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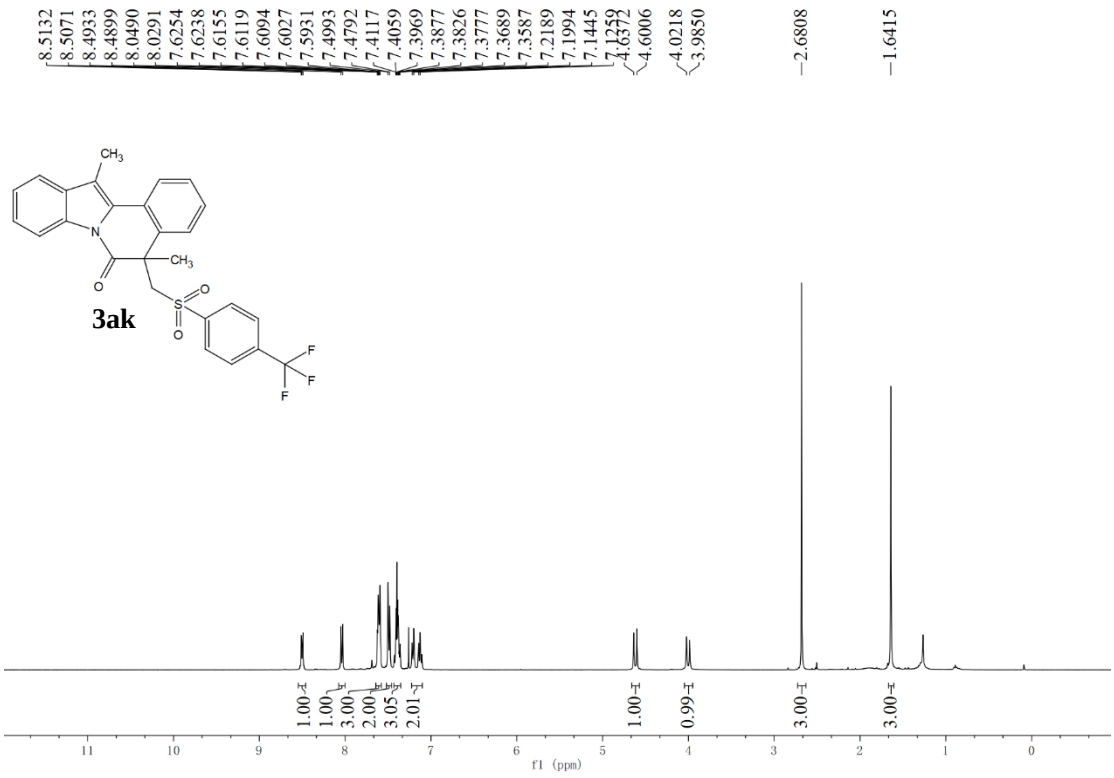
127.18
126.29
126.12
125.16
124.63
118.62
116.88
115.37
101.59
64.46
46.44
31.75
11.75
CH3
CH3
O
N
O
S
O
O
I
3aj
f1 (ppm)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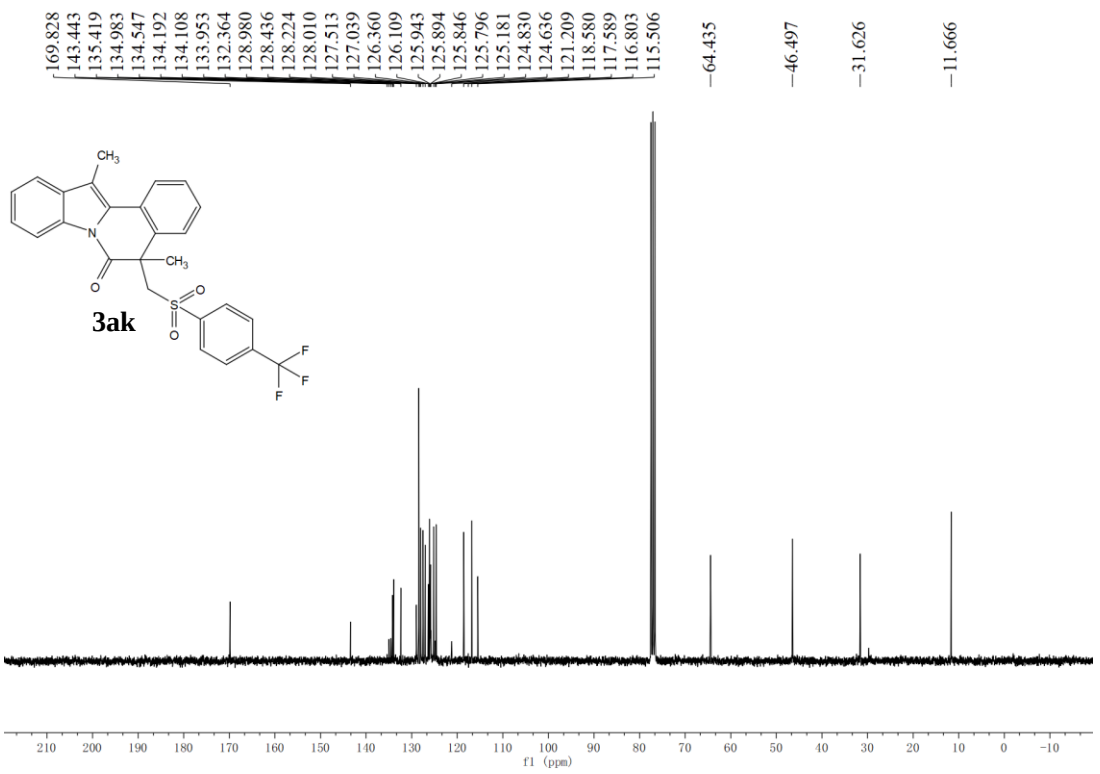
7.6155
7.6119
7.6094
7.6027
7.5931
7.4993
7.4792
7.4117
7.4059
7.3969
7.3877
7.3826
7.3777
7.3689
7.3587
7.2189
7.1994
7.1445
7.1259
4.6372
4.6006
4.0218
3.9850
2.6808
1.6415
CH3
CH3
O
N
O
S
O
O
F
F
F
3ak
1.00
1.00
3.00
2.00
3.05
2.01
1.00
0.99
3.00
3.00
f1 (ppm)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128.436
128.224
128.010
127.513
127.039
126.360
126.109
125.943
125.894
125.846
125.796
125.181
124.830
124.636
121.209
118.580
117.589
116.803
115.506
64.435
46.497
31.626
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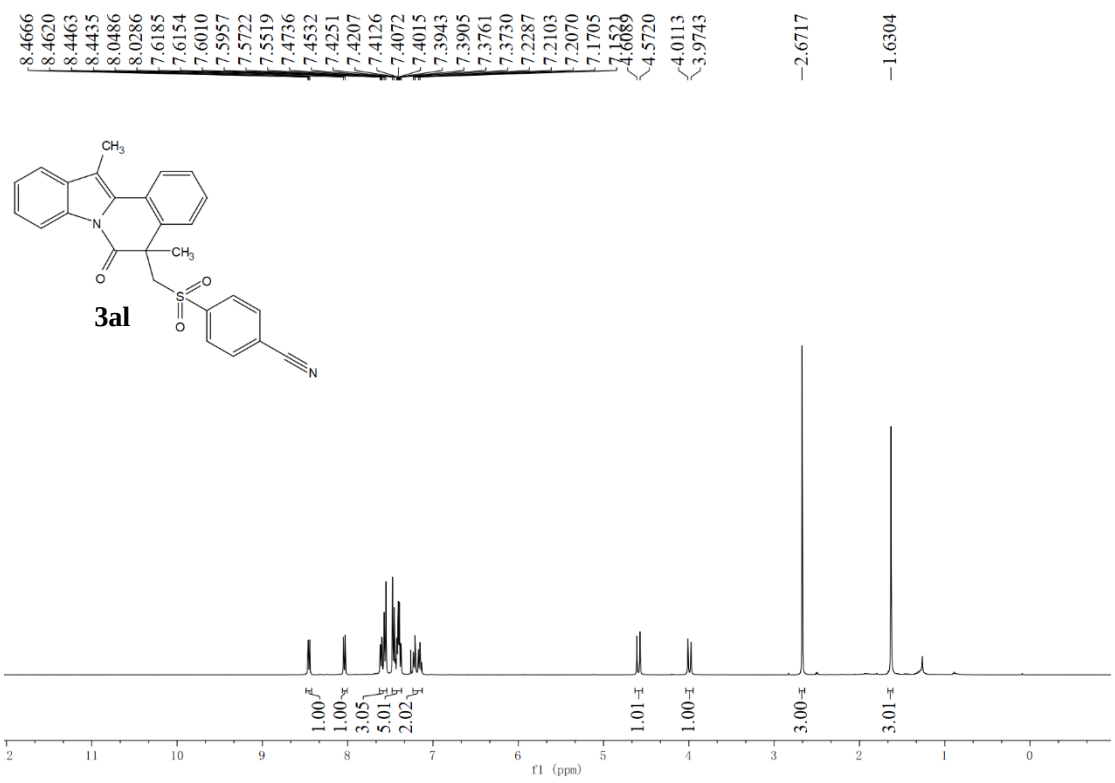
CH3
CH3
O
N
O
S
O
O
F
F
F
f1 (ppm)

3ak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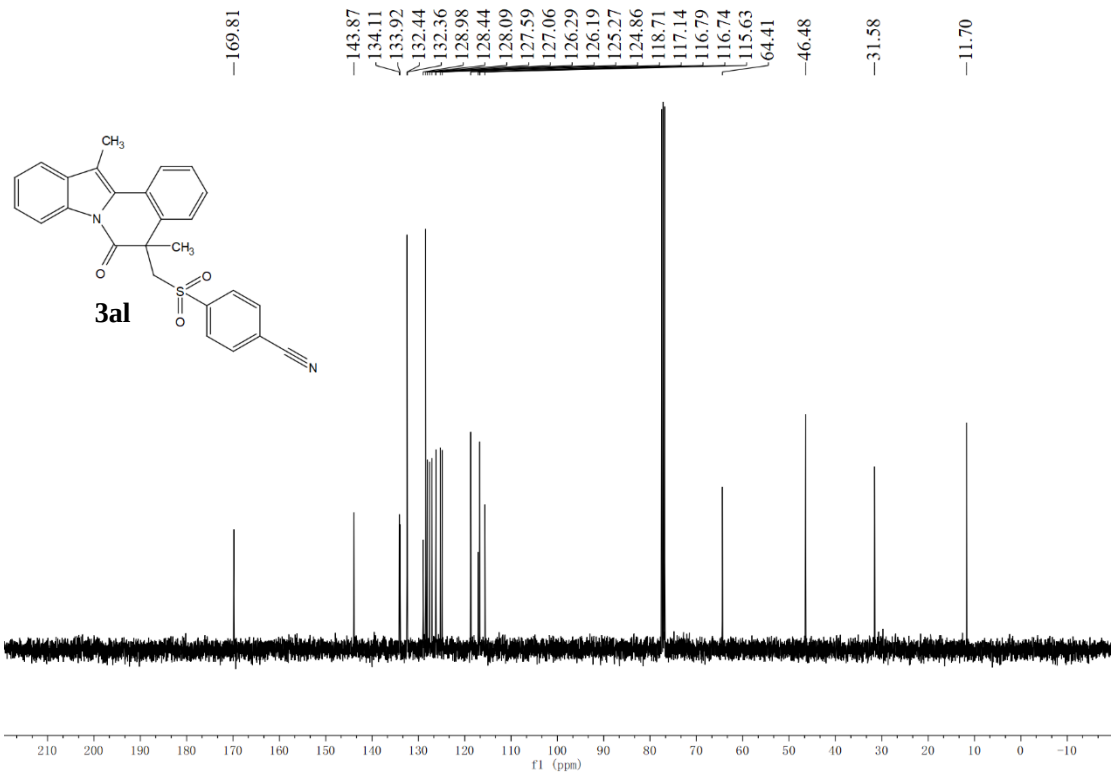
7.5722
7.5519
7.4736
7.4532
7.4251
7.4207
7.4126
7.4072
7.4015
7.3943
7.3905
7.3761
7.3730
7.2287
7.2103
7.2070
7.1705
7.1521
4.6089
4.5720
4.0113
3.9743
2.6717
1.6304
CH3
CH3
O
N
O
S
O
O
N
1.00
1.00
3.05
5.01
2.02
1.01
1.00
3.00
3.01
f1 (ppm)

3al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132.36
128.98
128.44
128.09
127.59
127.06
126.29
126.19
125.27
124.86
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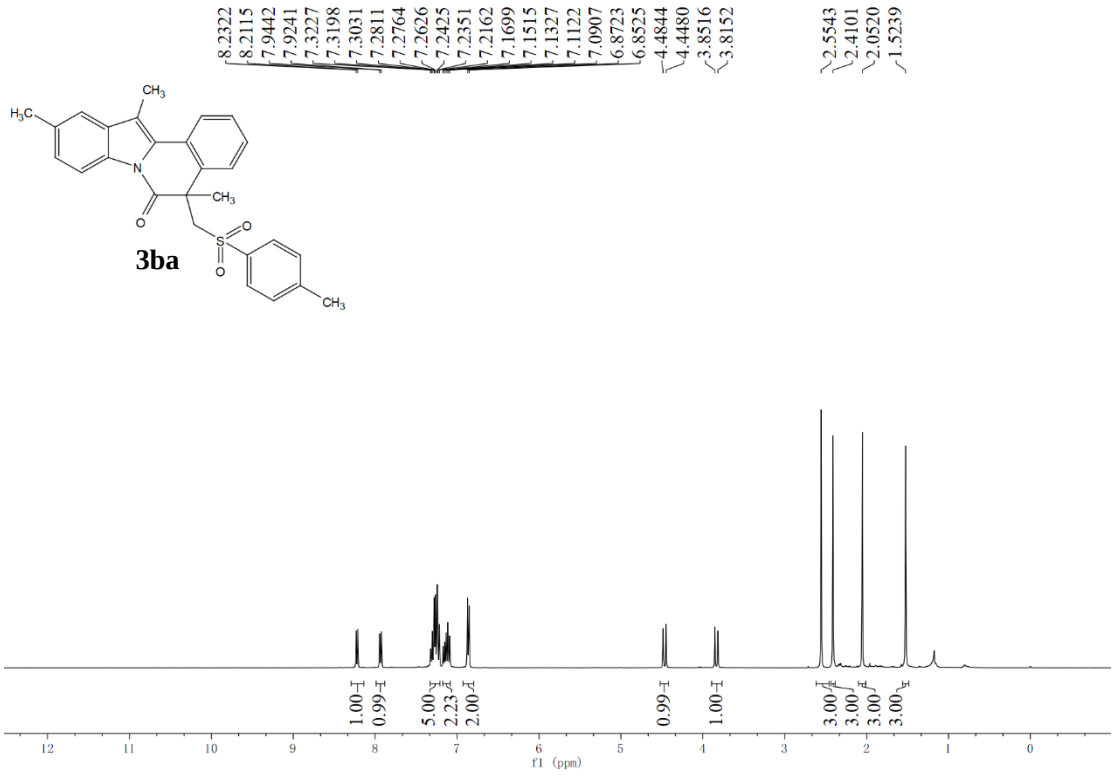
117.14
116.79
116.74
115.63
64.41
46.48
31.58
11.70
3al
f1 (ppm)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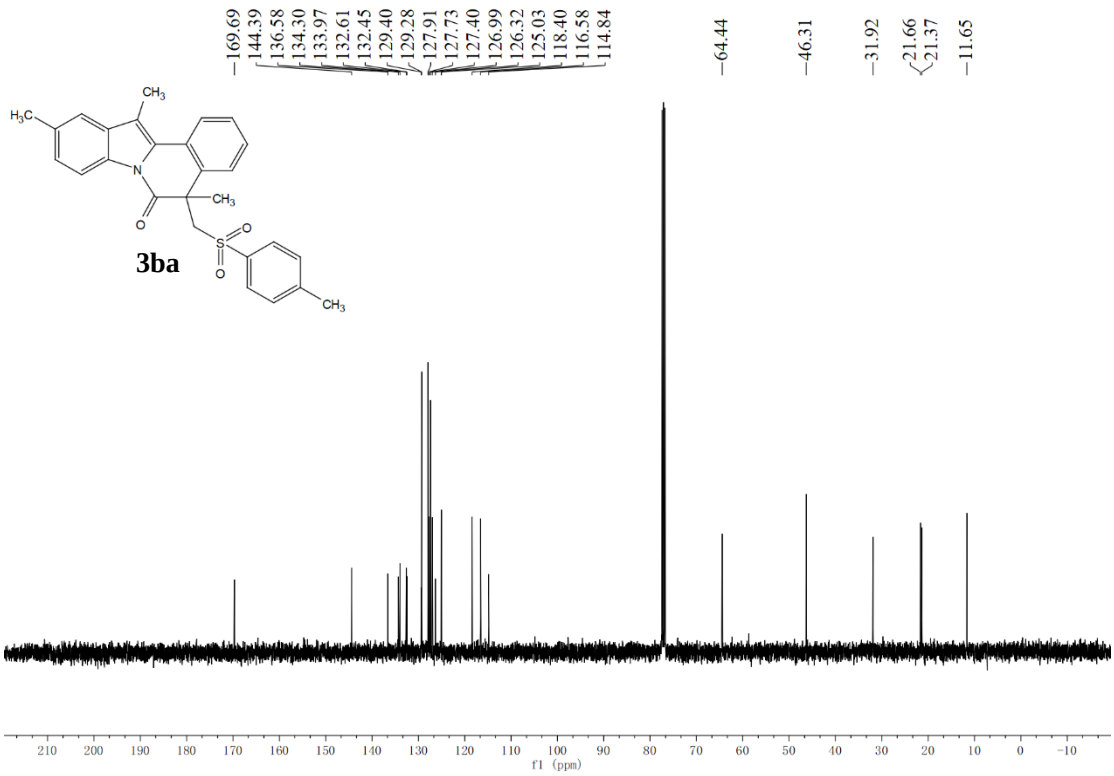
7.9442
7.9241
7.3227
7.3198
7.3031
7.2811
7.2764
7.2626
7.2425
7.2351
7.2162
7.1699
7.1515
7.1327
7.1122
7.0907
6.8723
6.8525
4.4844
4.4480
3.8516
3.8152
2.5543
2.4101
2.0520
1.5239
3ba
1.00
0.99
5.00
2.23
2.00
0.99
1.00
3.00
3.00
3.00
3.00
f1 (ppm)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132.61
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129.40
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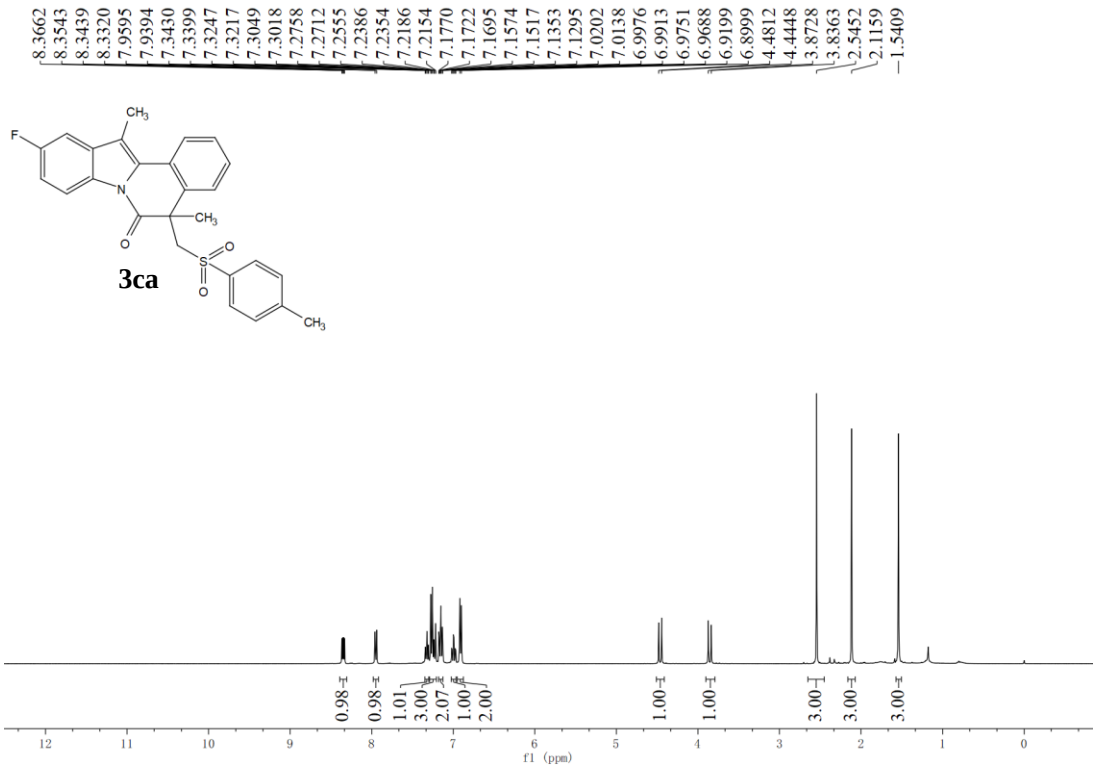
127.91
127.73
127.40
126.99
126.32
125.03
118.40
116.58
114.84
64.44
46.31
31.92
21.66
21.37
11.65
3ba
f1 (ppm)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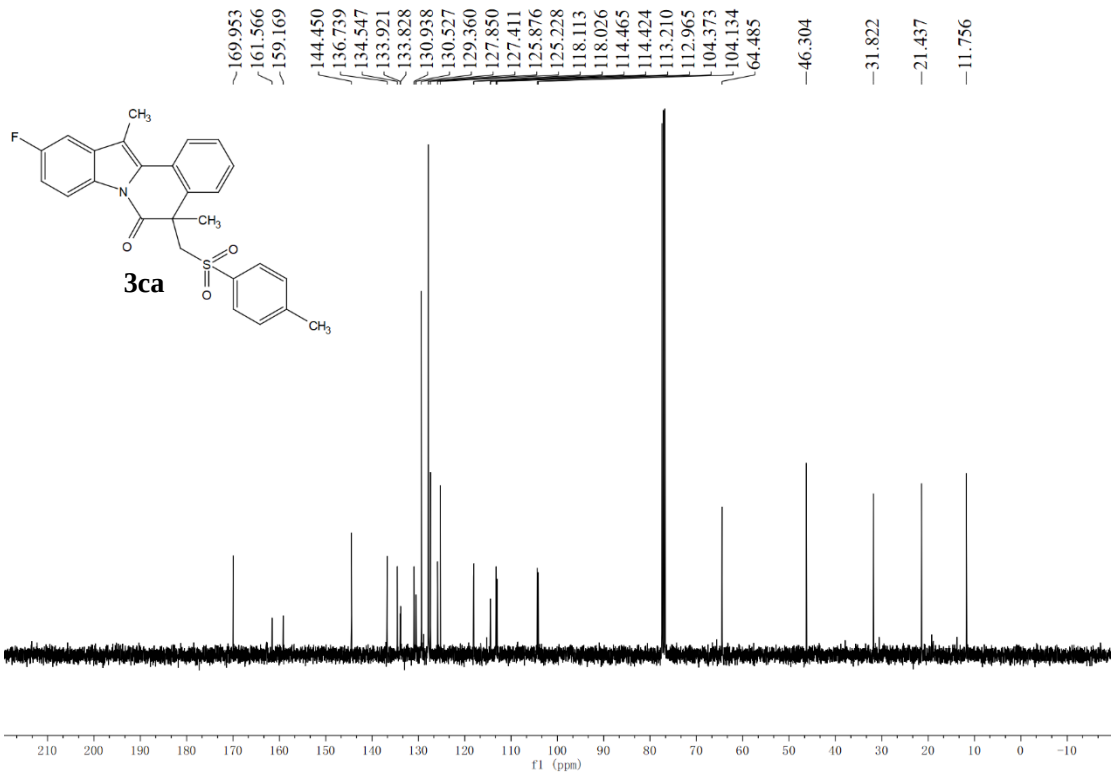
7.3399
7.3247
7.3217
7.3049
7.3018
7.2758
7.2712
7.2555
7.2386
7.2354
7.2186
7.2154
7.1770
7.1722
7.1695
7.1574
7.1517
7.1353
7.1295
7.0202
7.0138
6.9976
6.9913
6.9751
6.9688
6.9199
6.8999
4.4812
4.4448
3.8728
3.8363
2.5452
2.1159
1.5409
3ca
0.98
0.98
1.01
3.00
2.07
1.00
2.00
1.00
1.00
3.00
3.00
3.00
f1 (ppm)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136.739
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133.921
133.828
130.938
130.527
129.360
127.850
127.411
125.876
125.228
118.113
118.026
114.465
114.424
113.210
112.965
104.373
104.134
64.485
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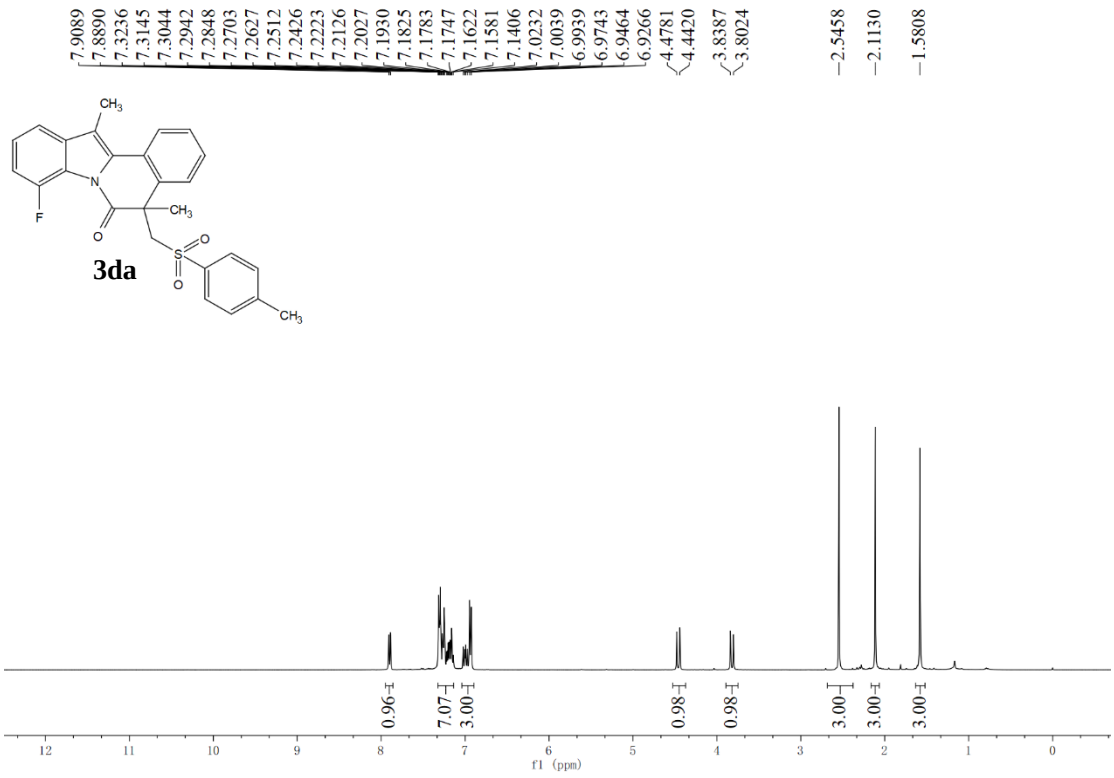
11.756
F
CH3
N
O
CH3
S
O
O
CH3
3ca
f1 (ppm)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7.3044
7.2942
7.2848
7.2703
7.2627
7.2512
7.2426
7.2223
7.2126
7.2027
7.1930
7.1825
7.1783
7.1747
7.1622
7.1581
7.1406
7.1232
7.0039
6.9939
6.9743
6.9464
6.9266
4.4781
4.4420
3.8387
3.8024
2.5458
2.1130
1.5808
CH3
N
F
O
CH3
S
O
O
CH3
3da
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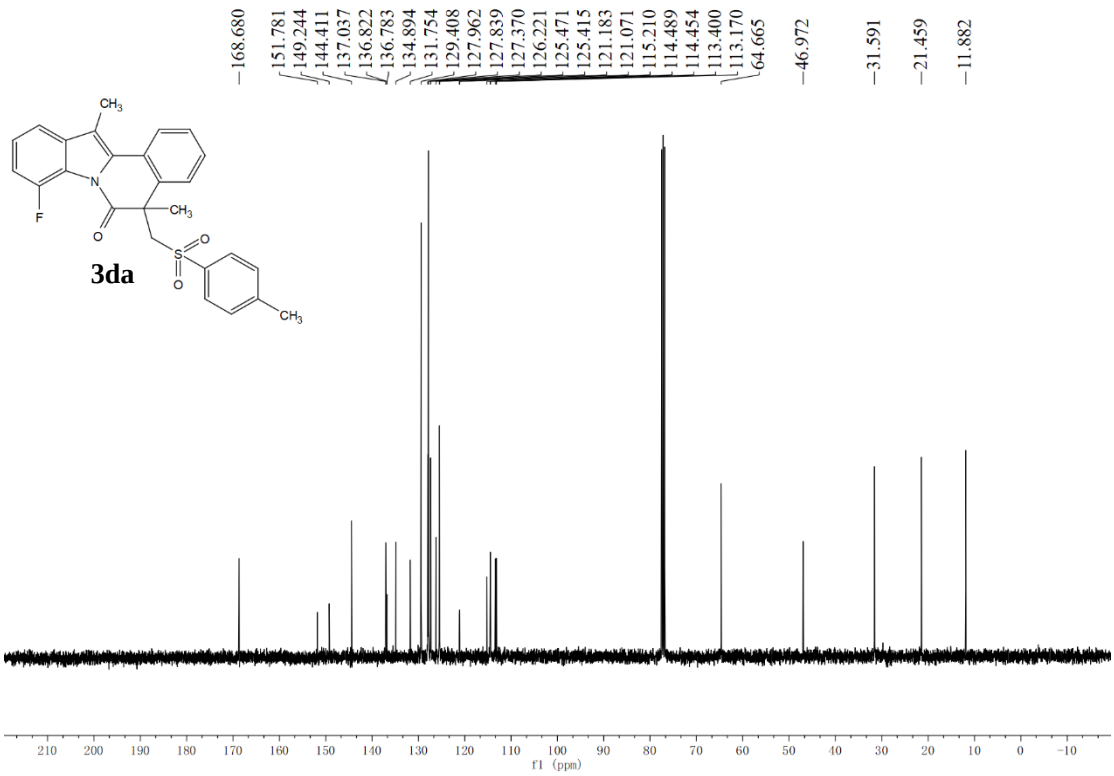
7.07
3.00
0.98
0.98
3.00
3.00
3.00
f1 (ppm)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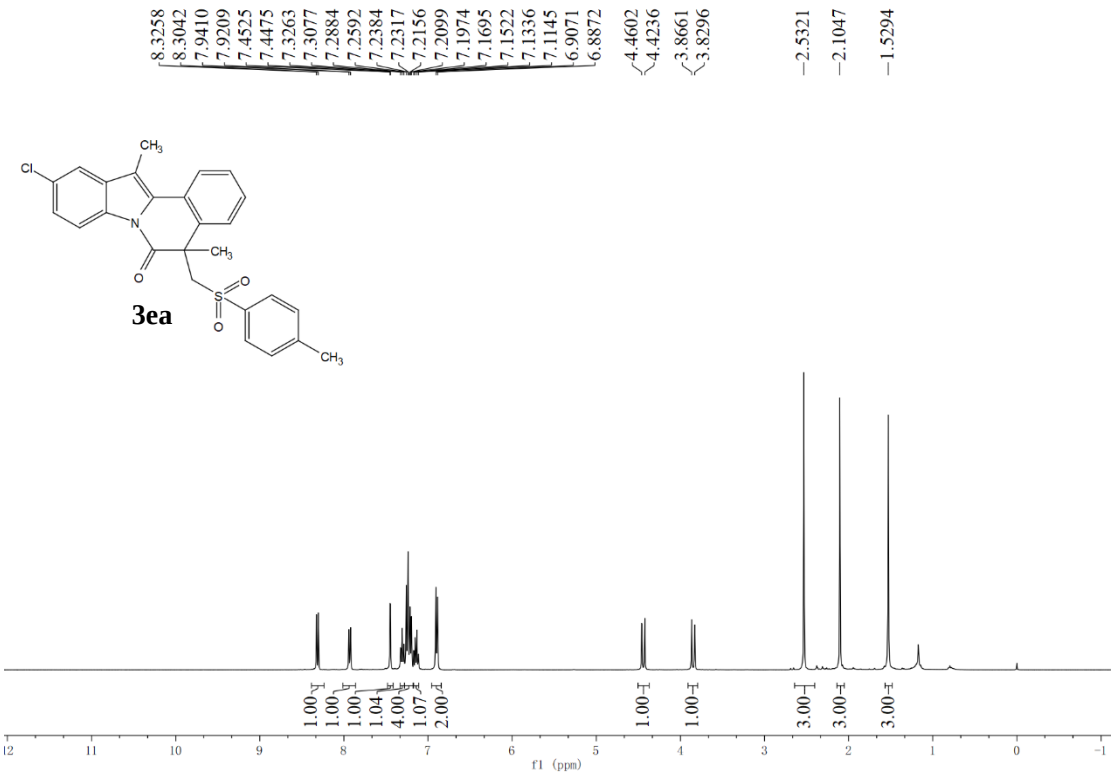
136.783
134.894
131.754
129.408
127.962
127.839
127.370
126.221
125.471
125.415
121.183
121.071
115.210
114.489
114.454
113.400
113.170
64.665
46.972
31.591
21.459
11.882
3da
f1 (ppm)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7.3263
7.3077
7.2884
7.2592
7.2384
7.2317
7.2156
7.2099
7.1974
7.1695
7.1522
7.1336
7.1145
6.9071
6.8872
4.4602
4.4236
3.8661
3.8296
2.5321
2.1047
1.5294
1.00
1.00
1.00
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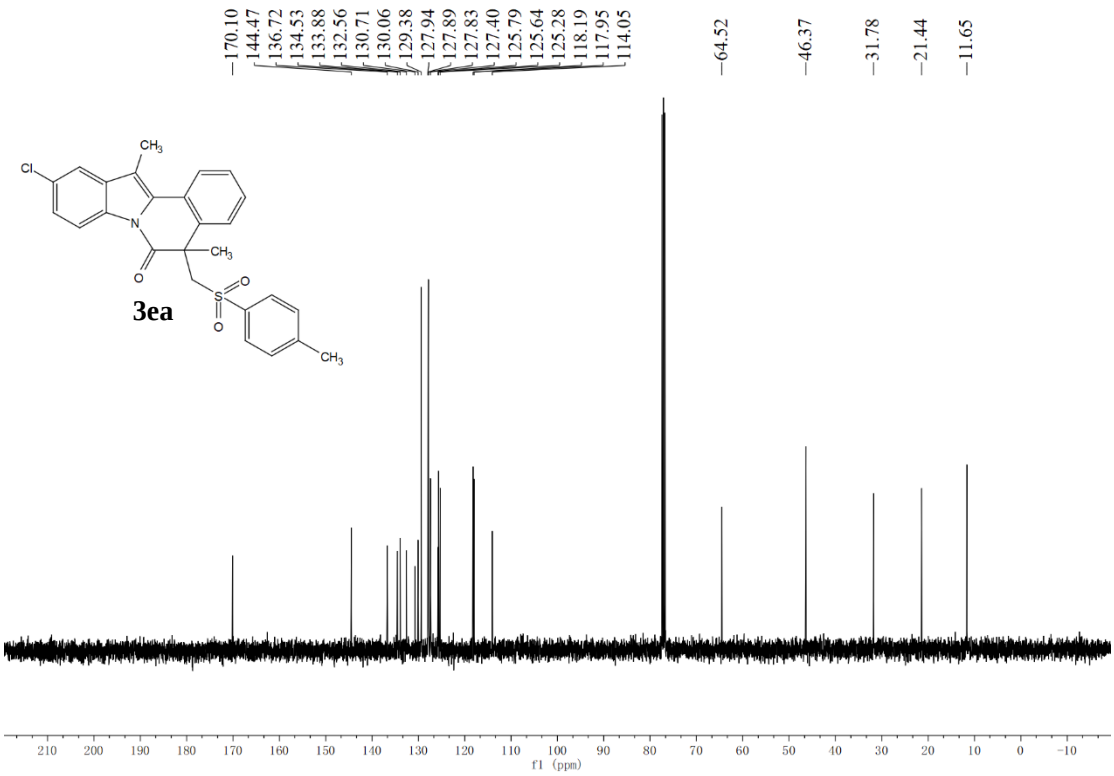
4.00
1.07
2.00
1.00
1.00
3.00
3.00
3.00
3ea
f1 (ppm)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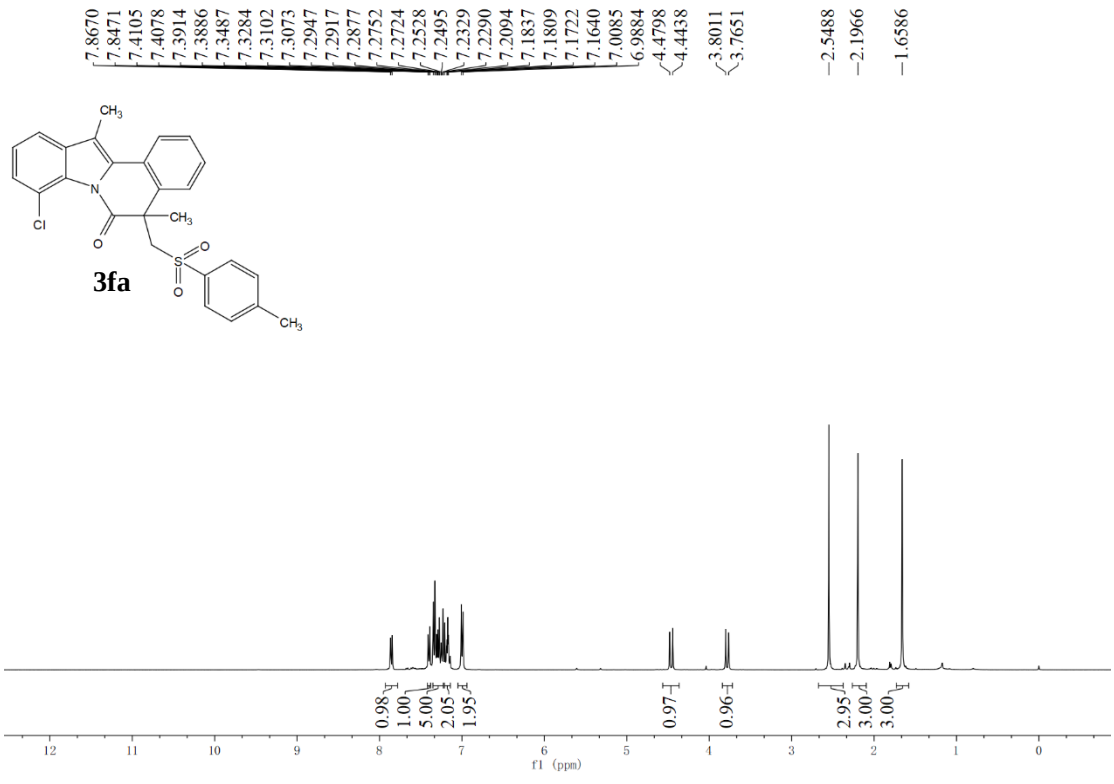
144.47
136.72
134.53
133.88
132.56
130.71
130.06
129.38
127.94
127.89
127.83
127.40
125.79
125.64
125.28
118.19
117.95
114.05
64.52
46.37
31.78
21.44
11.65
Cl
CH3
N
O
CH3
S
O
O
CH3
3ea
f1 (ppm)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7.3102
7.3073
7.2947
7.2917
7.2877
7.2752
7.2724
7.2528
7.2495
7.2329
7.2290
7.2094
7.1837
7.1809
7.1722
7.1640
7.0085
6.9884
4.4798
4.4438
3.8011
3.7651
2.5488
2.1966
1.6586
CH3
Cl
N
O
CH3
S
O
O
CH3
3fa
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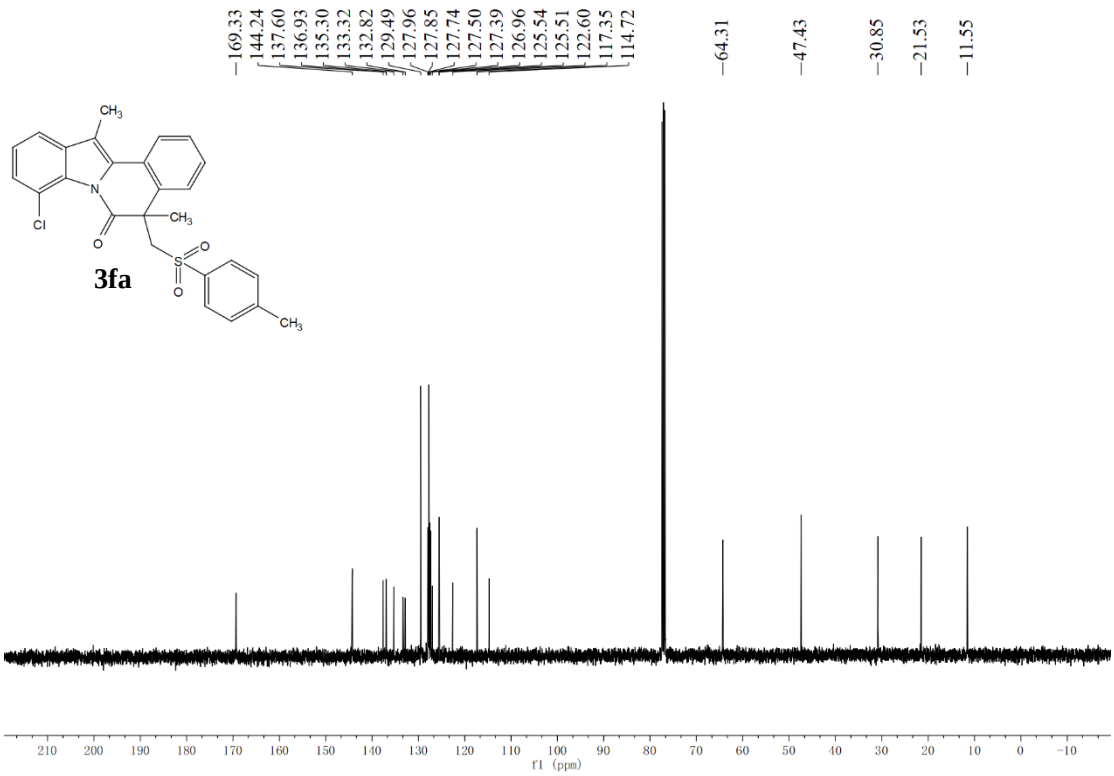
5.00
2.05
1.95
0.97
0.96
2.95
3.00
3.00
f1 (ppm)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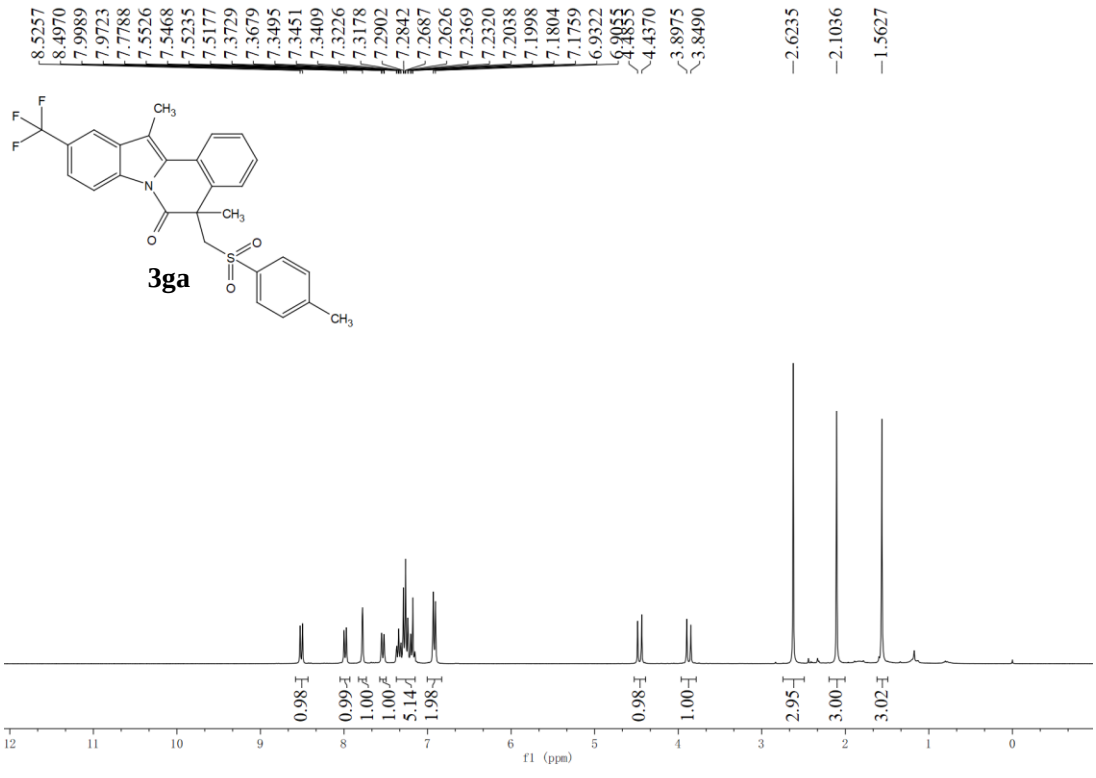
129.49
127.96
127.85
127.74
127.50
127.39
126.96
125.54
125.51
122.60
117.35
114.72
64.31
47.43
30.85
21.53
11.55
CH3
Cl
N
O
CH3
S
O
O
CH3
f1 (ppm)

3fa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7.5177
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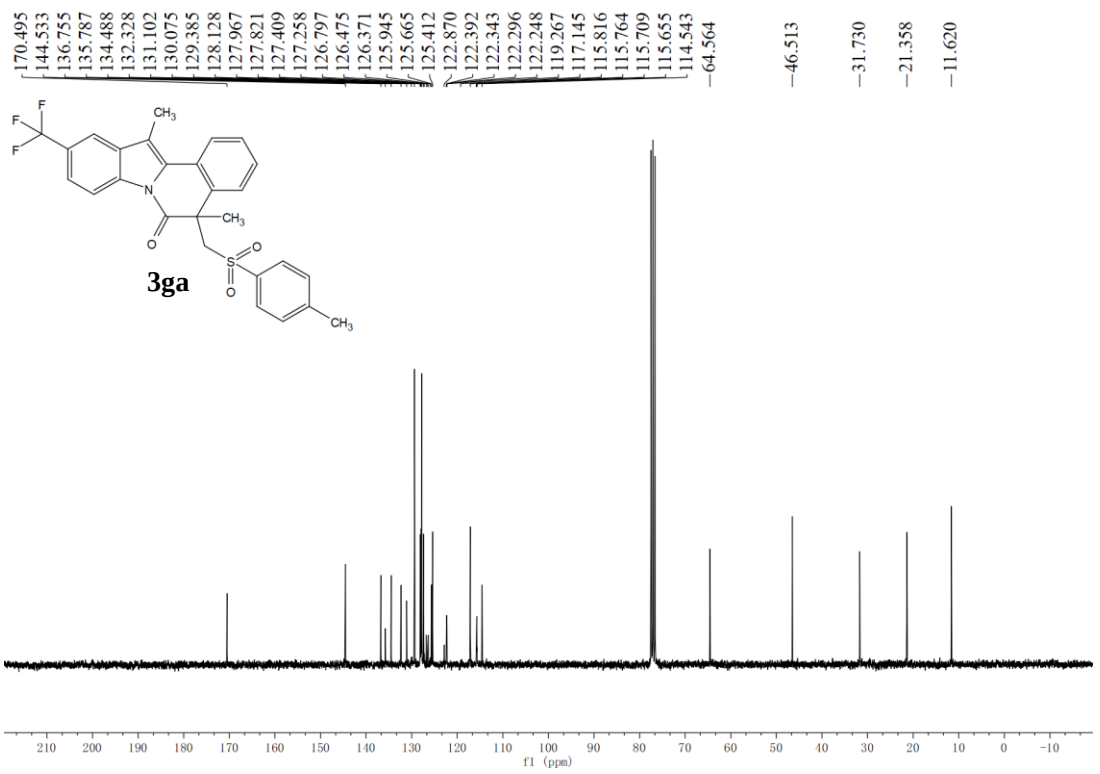
7.3679
7.3495
7.3451
7.3409
7.3226
7.3178
7.2902
7.2842
7.2687
7.2626
7.2369
7.2320
7.2038
7.1998
7.1804
7.1759
6.9322
4.4855
4.4370
3.8975
3.8490
2.6235
2.1036
1.5627
F
F
F
CH3
N
O
CH3
S
O
O
CH3
0.98
0.99
1.00
1.00
5.14
1.98
0.98
1.00
2.95
3.00
3.02
f1 (ppm)

3ga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127.967
127.821
127.409
127.258
126.797
126.475
126.371
125.945
125.665
125.412
122.870
122.392
122.343
122.296
122.248
119.267
117.145
115.816
115.764
115.709
115.655
114.543
64.564
46.513
31.730
21.358
11.620
F
F
F
CH3
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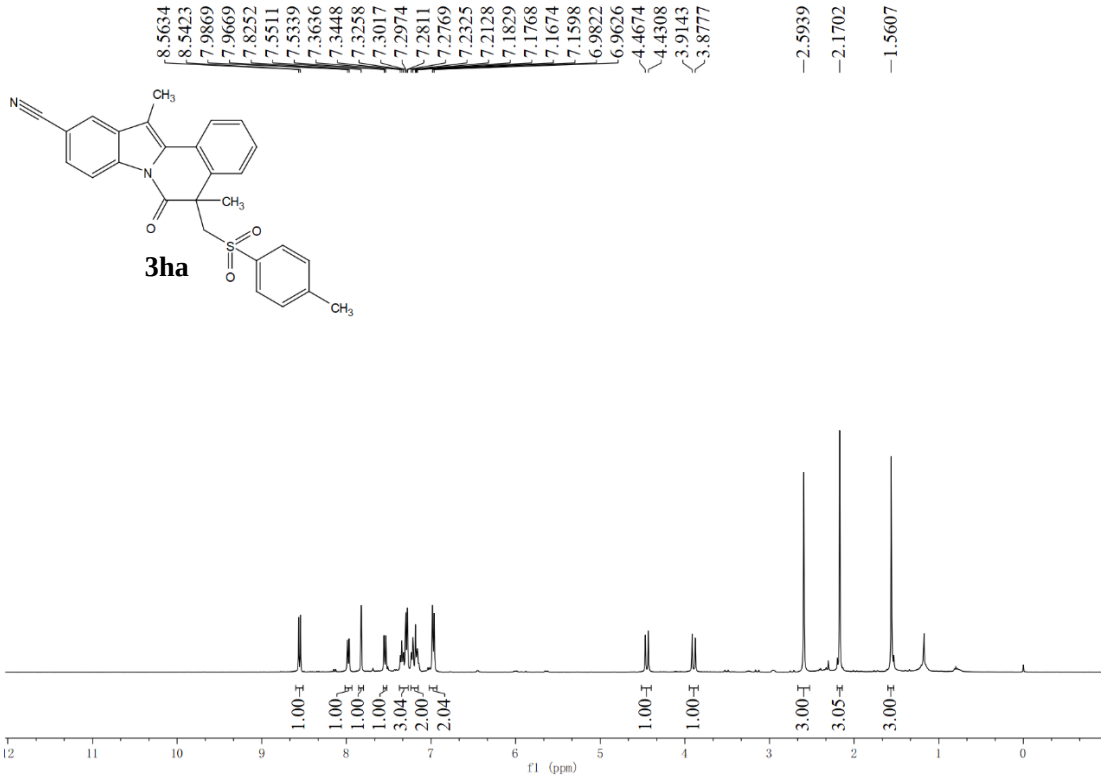
O
CH3
O
S
O
O
CH3
3ga
f1 (ppm)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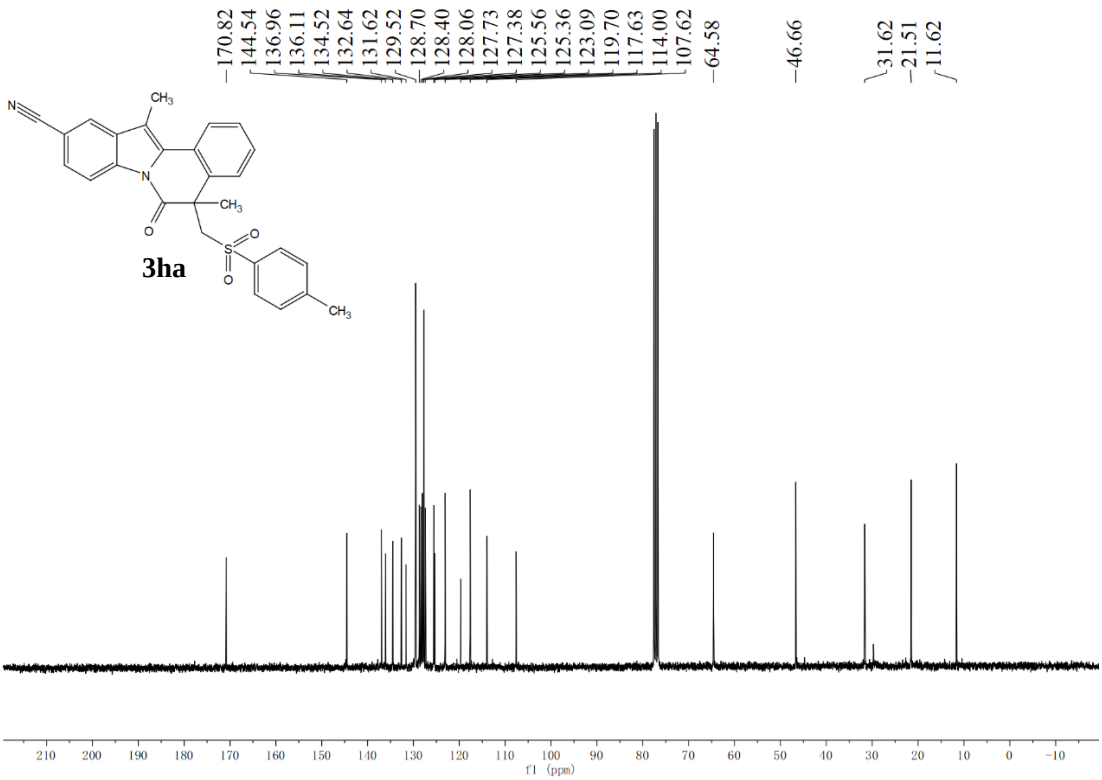
7.3017
7.2974
7.2811
7.2769
7.2325
7.2128
7.1829
7.1768
7.1674
7.1598
6.9822
6.9626
4.4674
4.4308
3.9143
3.8777
2.5939
2.1702
1.5607
N
CH3
N
O
CH3
O
S
O
O
CH3
3ha
1.00
1.00
1.00
3.04
2.00
2.04
1.00
1.00
3.00
3.05
3.00
f1 (ppm)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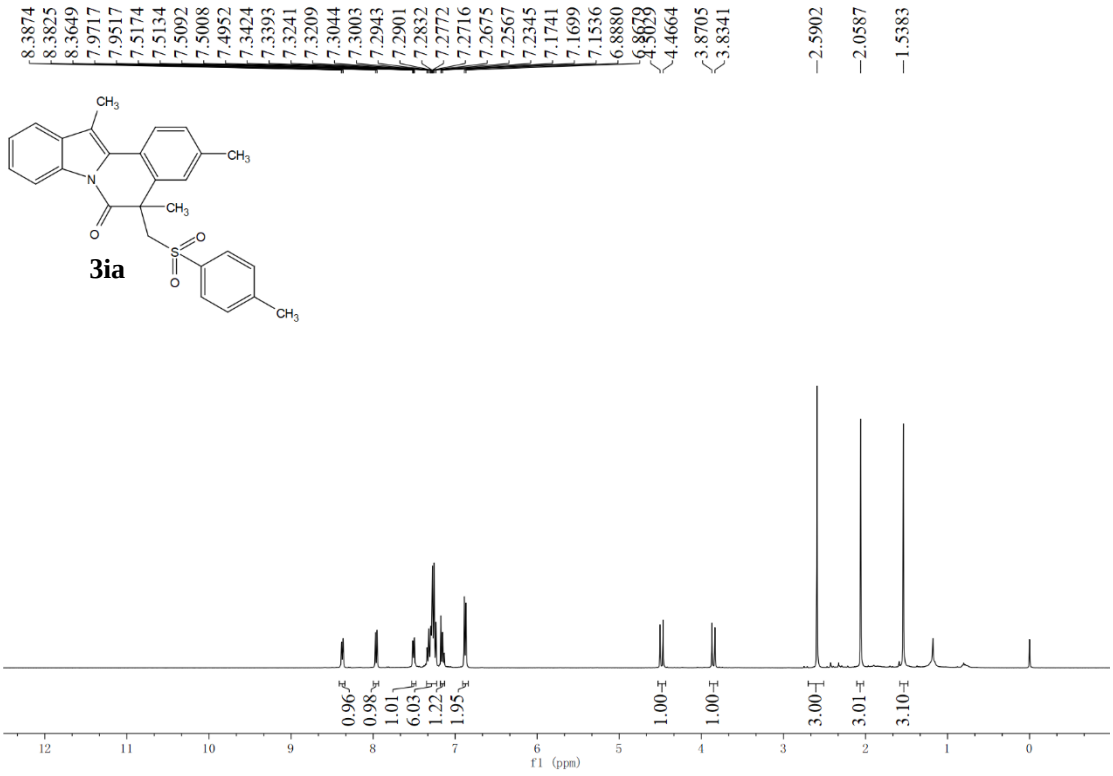
134.52
132.64
131.62
129.52
128.70
128.40
128.06
127.73
127.38
125.56
125.36
123.09
119.70
117.63
114.00
107.62
64.58
46.66
31.62
21.51
11.62
3ha
f1 (ppm)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7.3241
7.3209
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7.3003
7.2943
7.2901
7.2832
7.2772
7.2716
7.2675
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7.2345
7.1741
7.1699
7.1536
6.8880
4.4664
3.8705
3.8341
2.5902
2.0587
1.5383
3ia
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0.98
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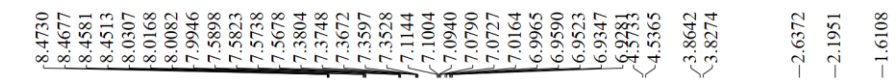
6.03
1.22
1.95
1.00
1.00
3.00
3.01
3.10
f1 (ppm)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7.5678
7.3804
7.3748
7.3672
7.3597
7.3528
7.1144
7.1004
7.0940
7.0790
7.0727
7.0164
6.9965
6.9590
6.9523
6.9347
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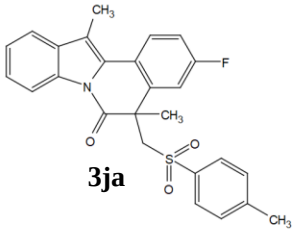
4.5365
3.8642
3.8274
2.6372
2.1951
1.6108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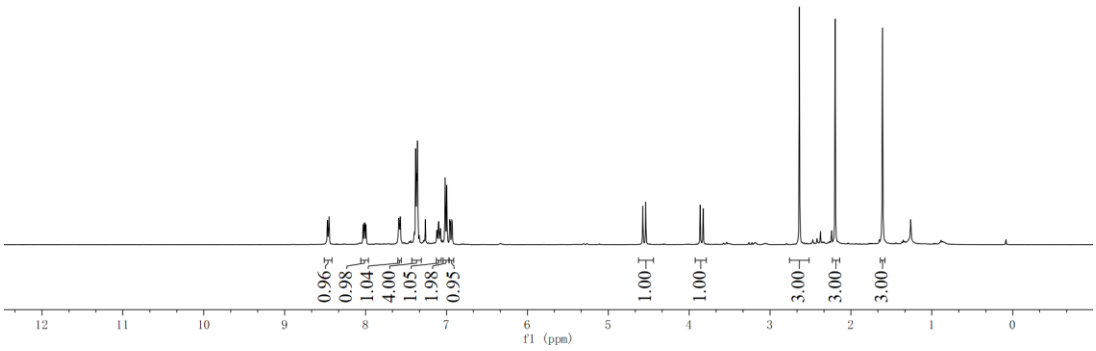
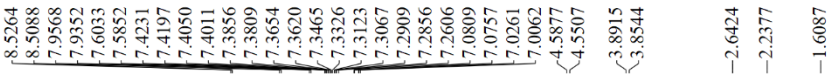
F
N
CH3
O
S
O
O
CH3

3ja


0.96
0.98
1.04
4.00
1.05
1.98
0.95
1.00
1.00
3.00
3.00
3.00
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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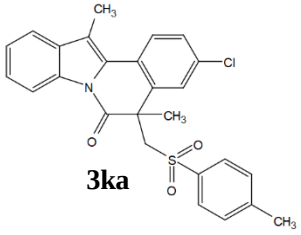
8.5088
7.9568
7.9352
7.6033
7.5852
7.4231
7.4197
7.4050
7.4011
7.3856
7.3809
7.3654
7.3620
7.3465
7.3326
7.3123
7.3067
7.2909
7.2856
7.2606
7.0809
7.0757
7.0261
7.0062
4.5877
4.5507
3.8915
3.8544
2.6424
2.2377
1.6087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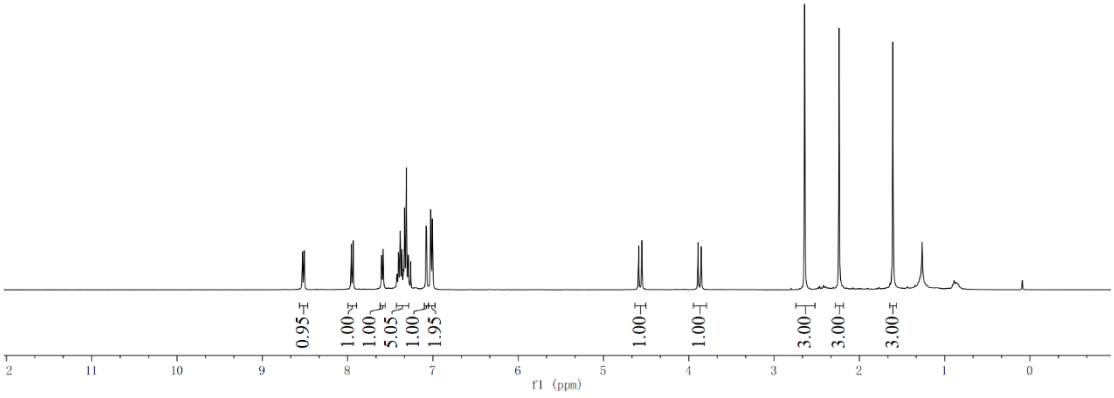
Cl
N
CH3
O
S
O
O
CH3

3ka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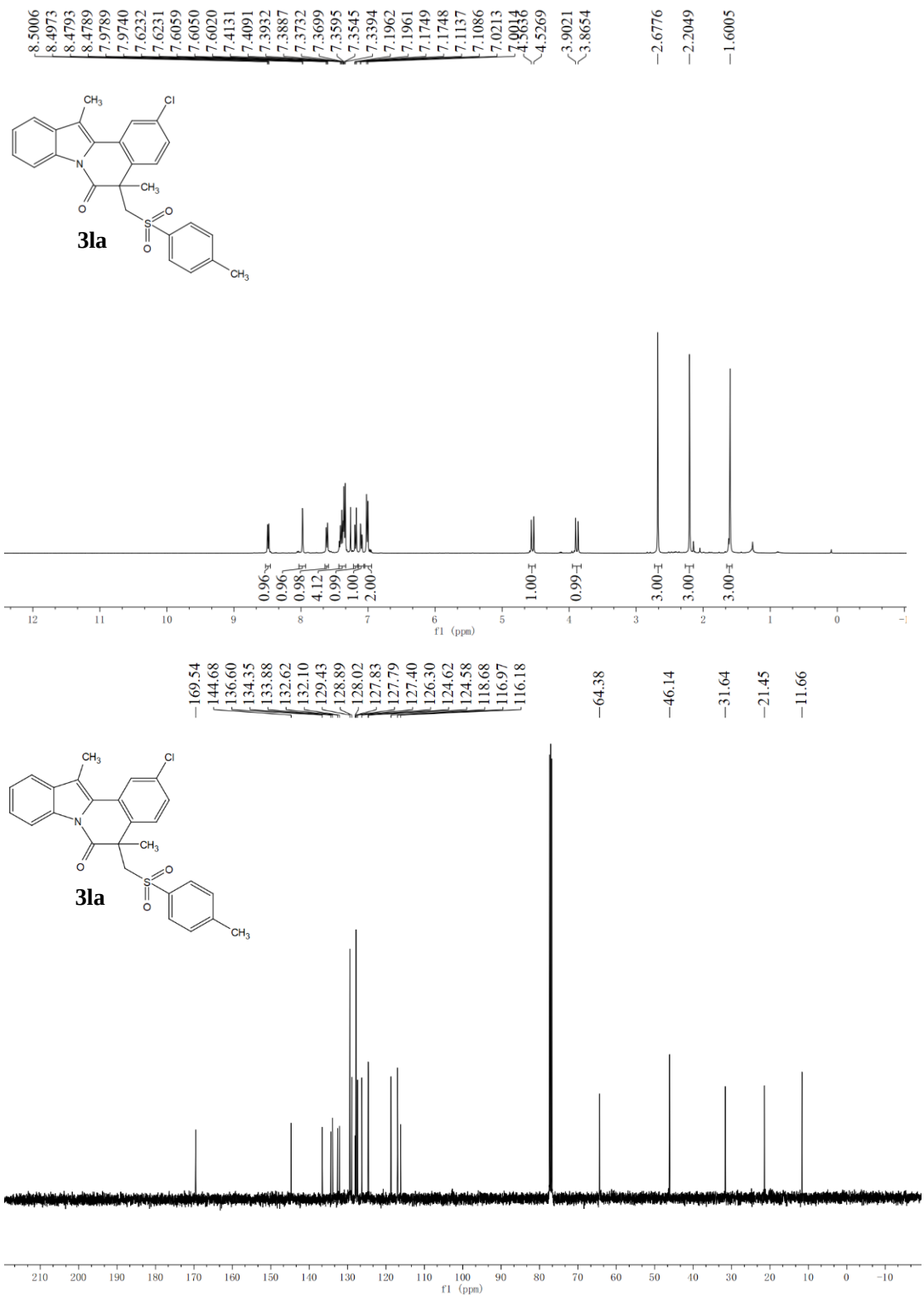
1.00
1.00
5.05
1.00
1.95
1.00
1.00
3.00
3.00
3.00
2
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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8.4793
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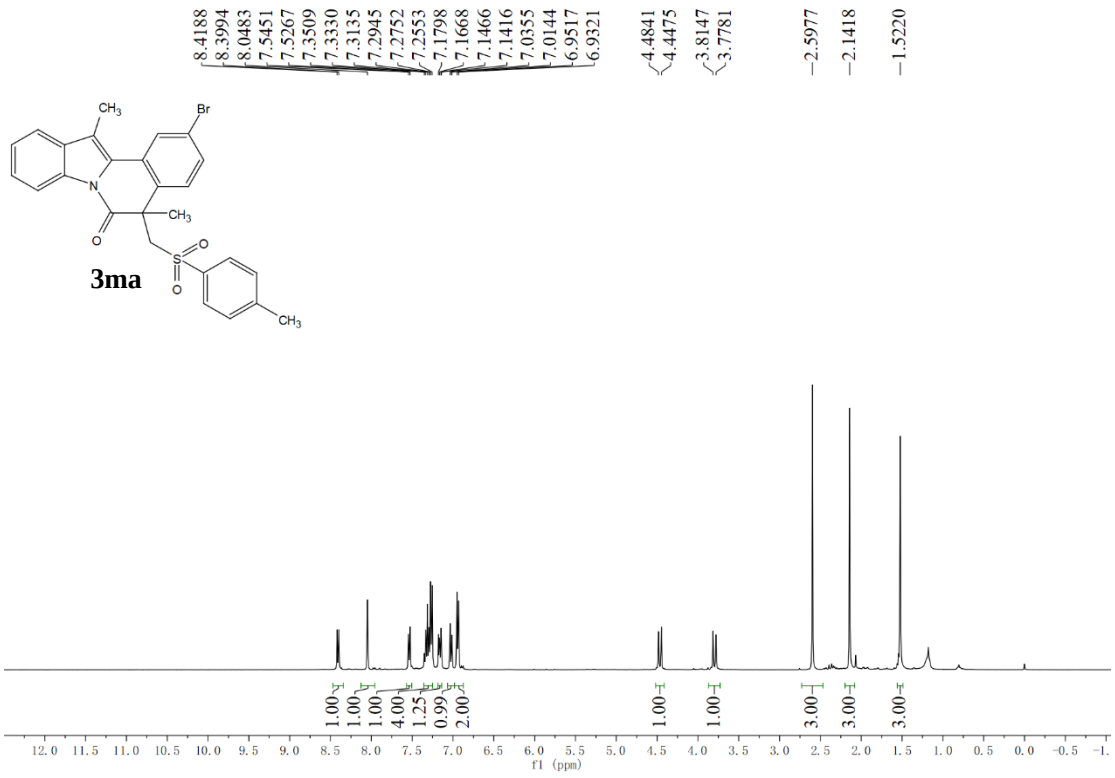
7.9789
7.9740
7.6232
7.6231
7.6059
7.6050
7.6020
7.4131
7.4091
7.3932
7.3887
7.3732
7.3699
7.3595
7.3545
7.3394
7.1962
7.1961
7.1749
7.1748
7.1137
7.1086
7.0213
4.5269
3.9021
3.8654
2.6776
2.2049
1.6005
CH3
Cl
N
O
CH3
S
O
O
CH3
3la
0.96
0.96
0.98
4.12
0.99
1.00
2.00
1.00
0.99
3.00
3.00
3.00
f1 (ppm)
169.54
144.68
136.60
134.35
133.88
132.62
132.10
129.43
128.89
128.02
127.83
127.79
127.40
126.30
124.62
124.58
118.68
116.97
116.18
64.38
46.14
31.64
21.45
11.66
f1 (ppm)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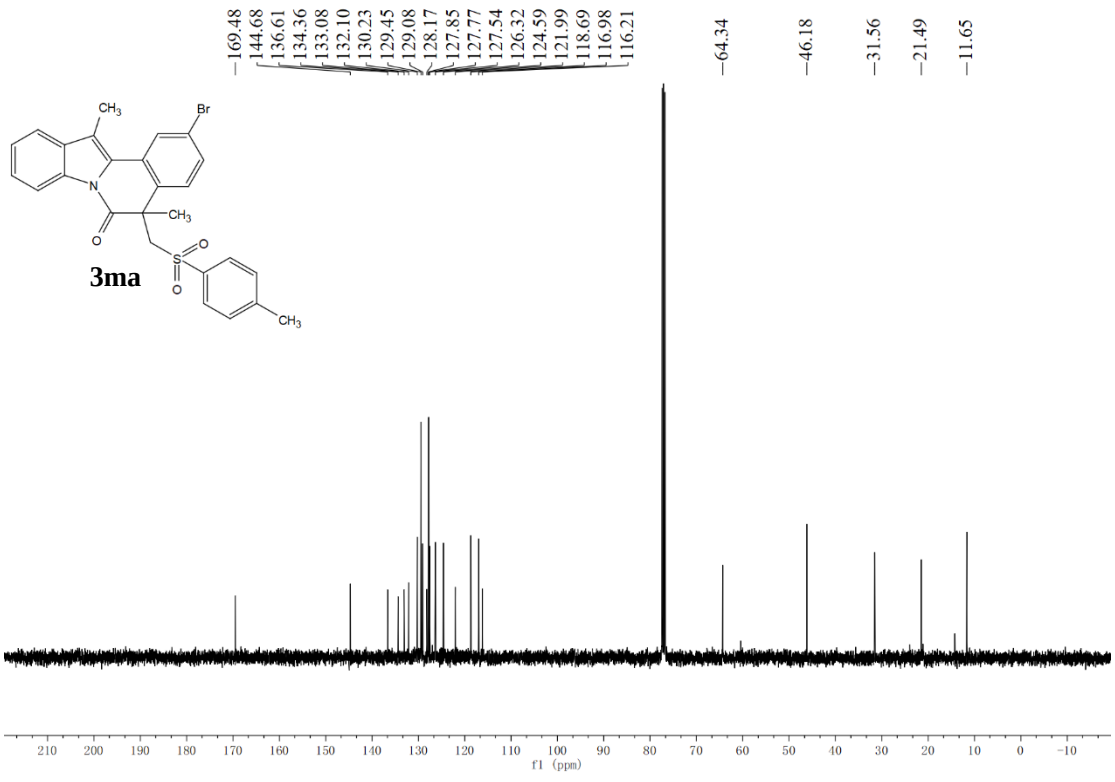
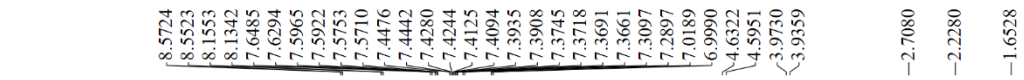
8.3994
8.0483
7.5451
7.5267
7.3509
7.3330
7.3135
7.2945
7.2752
7.2553
7.1798
7.1668
7.1466
7.1416
7.0355
7.0144
6.9517
6.9321
4.4841
4.4475
3.8147
3.7781
2.5977
2.1418
1.5220
3ma
1.00
1.00
1.00
4.00
1.25
0.99
2.00
1.00
1.00
3.00
3.00
3.00
f1 (ppm)


169.48
144.68
136.61
134.36
133.08
132.10
130.23
129.45
129.08
128.17
127.85
127.77
127.54
126.32
124.59
121.99
118.69
116.98
116.21
64.34
46.18
31.56
21.49
11.65
3ma
f1 (ppm)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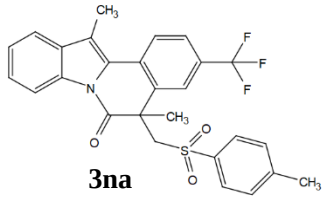
8.5523
8.1553
8.1342
7.6485
7.6294
7.5965
7.5922
7.5753
7.5710
7.4476
7.4442
7.4280
7.4244
7.4125
7.4094
7.3935
7.3908
7.3745
7.3718
7.3691
7.3661
7.3097
7.2897
7.0189
6.9990
4.6322
4.5951
3.9730
3.9359
2.7080
2.2280
1.6528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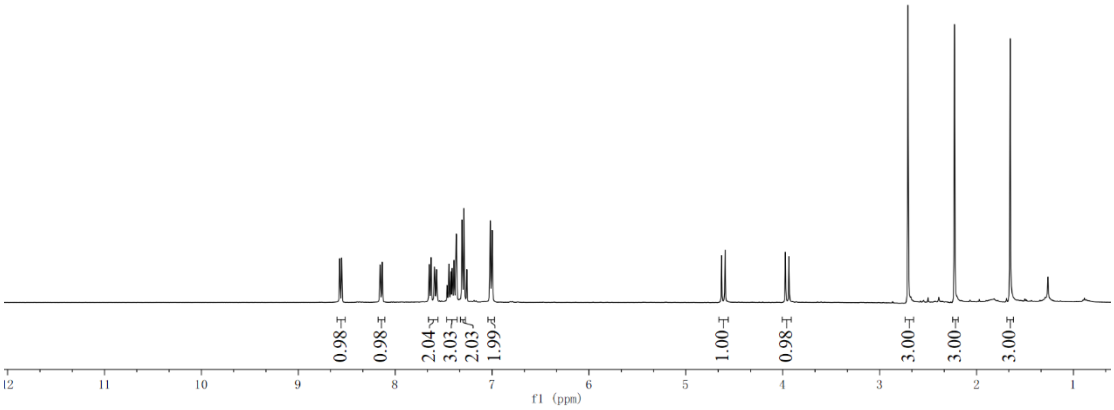
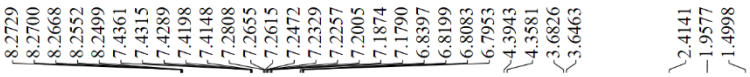
F
F
F
N
CH3
O
O
S
O
CH3

3na


0.98
0.98
2.04
3.03
2.03
1.99
1.00
0.98
3.00
3.00
3.00
f1 (ppm)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8.2700
8.2668
8.2552
8.2499
7.4361
7.4315
7.4289
7.4198
7.4148
7.2808
7.2655
7.2615
7.2472
7.2329
7.2257
7.2005
7.1874
7.1790
6.8397
6.8199
6.8083
6.7953
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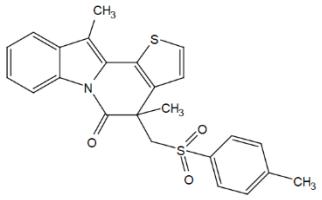
4.3581
3.6826
3.6463
2.4141
1.9577
1.4998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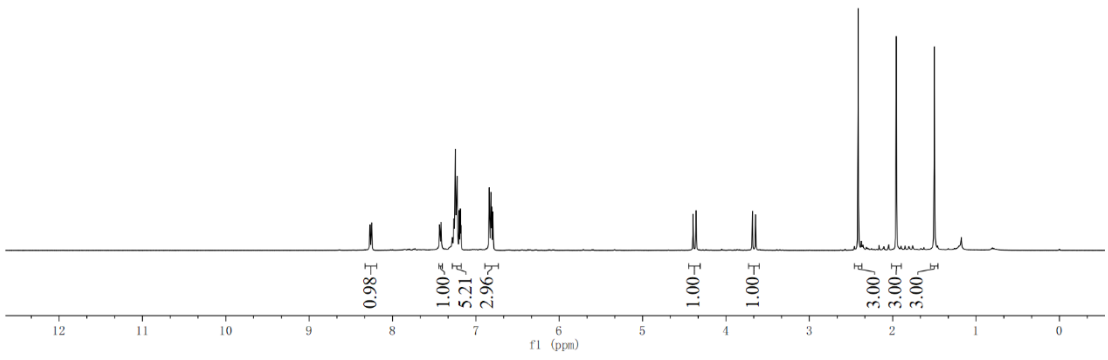
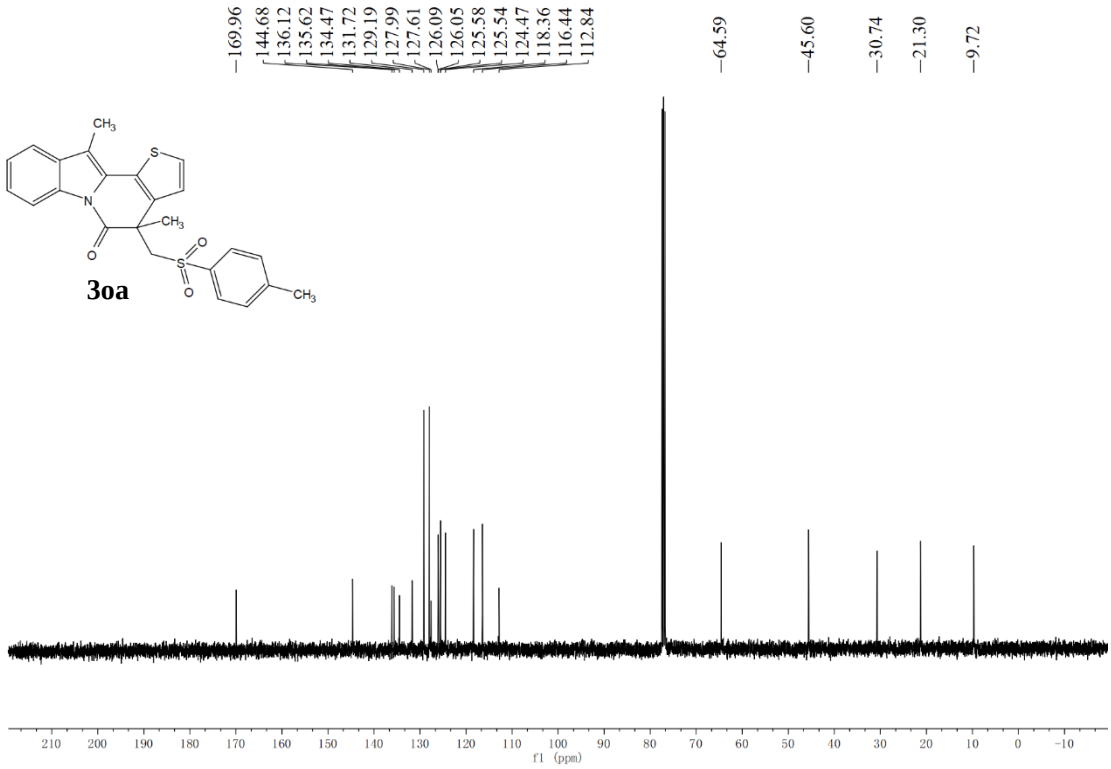
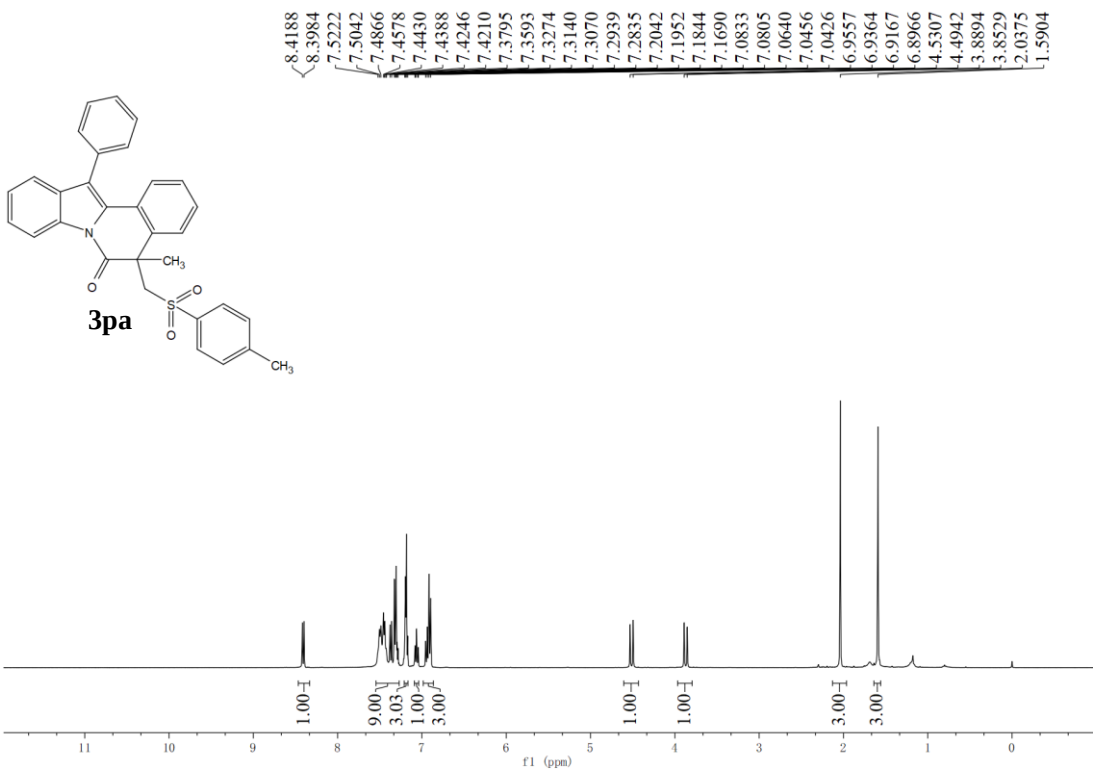
S
N
CH3
O
O
S
O
CH3

3oa


0.98
1.00
5.21
2.96
1.00
1.00
3.00
3.00
3.00
f1 (ppm)


169.96
144.68
136.12
135.62
134.47
131.72
129.19
127.99
127.61
126.09
126.05
125.58
125.54
124.47
118.36
116.44
112.84
64.59
45.60
30.74
21.30
9.72
f1 (ppm)

3oa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8.3984
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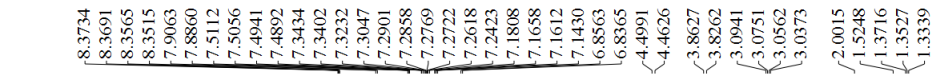
7.5042
7.4866
7.4578
7.4430
7.4388
7.4246
7.4210
7.3795
7.3593
7.3274
7.3140
7.3070
7.2939
7.2835
7.2042
7.1952
7.1844
7.1690
7.0833
7.0805
7.0640
7.0456
7.0426
6.9557
6.9364
6.9167
6.8966
4.5307
4.4942
3.8894
3.8529
2.0375
1.5904
1.00
9.00
3.03
1.00
3.00
1.00
1.00
3.00
3.00
f1 (ppm)

3pa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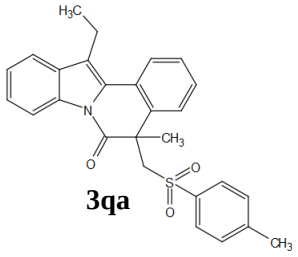
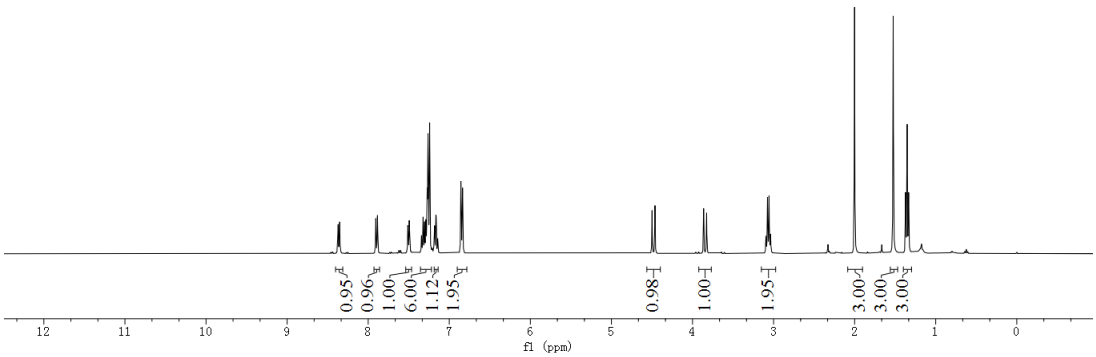
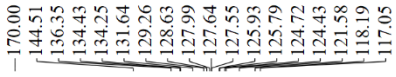
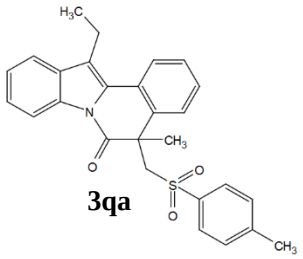
8.3691
8.3565
8.3515
7.9063
7.8860
7.5112
7.5056
7.4941
7.4892
7.3434
7.3402
7.3232
7.3047
7.2901
7.2858
7.2769
7.2722
7.2618
7.2423
7.1808
7.1658
7.1612
7.1430
6.8563
6.8365
4.4991
4.4626
3.8627
3.8262
3.0941
3.0751
3.0562
3.0373
2.0015
1.5248
1.3716
1.3527
1.3339


H3C
CH3
O
S
O
O
CH3

3qa

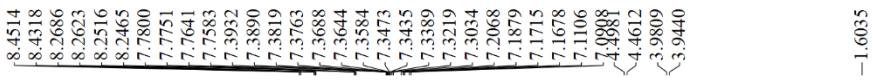

0.95
0.96
1.00
6.00
1.12
1.95
0.98
1.00
1.95
3.00
3.00
3.00
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


170.00
144.51
136.35
134.43
134.25
131.64
129.26
128.63
127.99
127.64
127.55
125.93
125.79
124.72
124.43
121.58
118.19
117.05
64.33
46.37
31.99
21.34
18.67
13.42


H3C
CH3
O
S
O
O
CH3

3qa

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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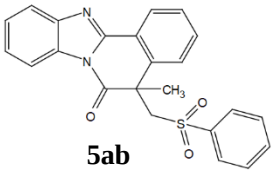
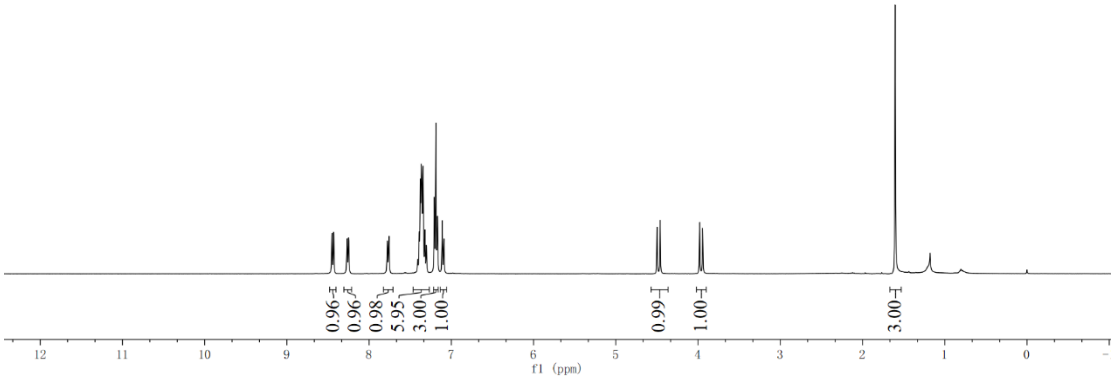
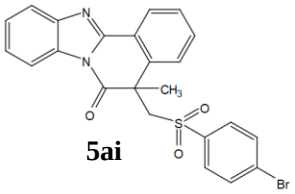
8.2686
8.2623
8.2516
8.2465
7.7800
7.7751
7.7641
7.7583
7.3932
7.3890
7.3819
7.3763
7.3688
7.3644
7.3584
7.3473
7.3435
7.3389
7.3219
7.3034
7.2068
7.1879
7.1715
7.1678
7.1106
4.4981
4.4612
3.9809
3.9440
1.6035


N
N
CH3
O
O
S
O
O

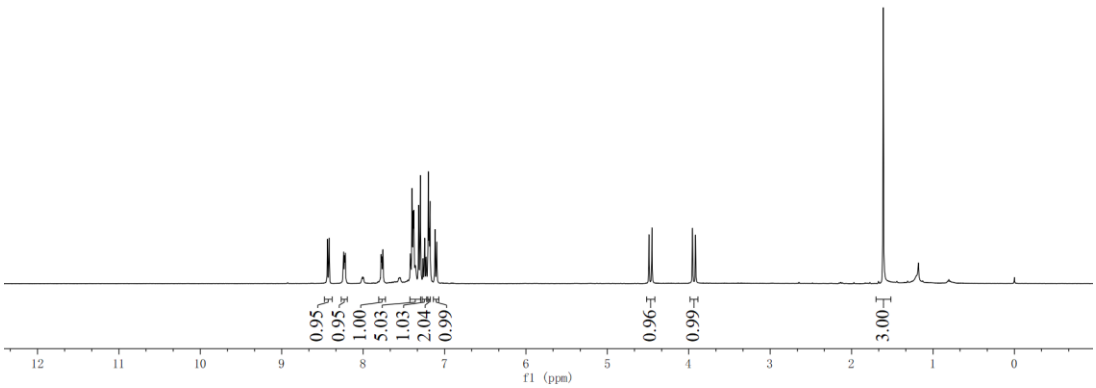
5ab


0.96
0.96
0.98
5.95
3.00
1.00
0.99
1.00
3.00
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


8.4375
8.4178
8.2406
8.2366
8.2286
8.2250
8.2176
7.7789
7.7720
7.7684
7.7590
7.7558
7.4194
7.4129
7.4012
7.3987
7.3958
7.3865
7.3781
7.3735
7.3601
7.3545
7.3486
7.3176
7.2969
7.2633
7.2440
7.2255
7.1995
7.1994
7.1891
7.1888
7.1785
7.1783
7.1161
7.0963
4.4890
4.4519
3.9540
3.9170
1.6108


N
N
CH3
O
O
S
O
Br

5ai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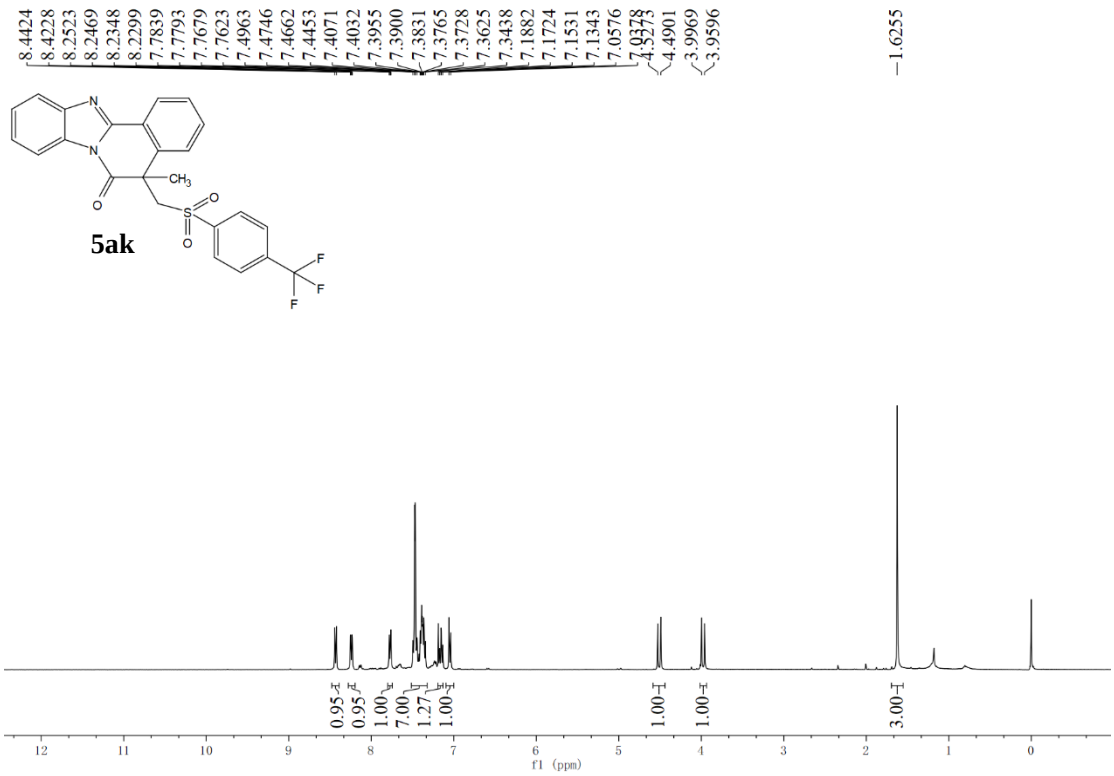
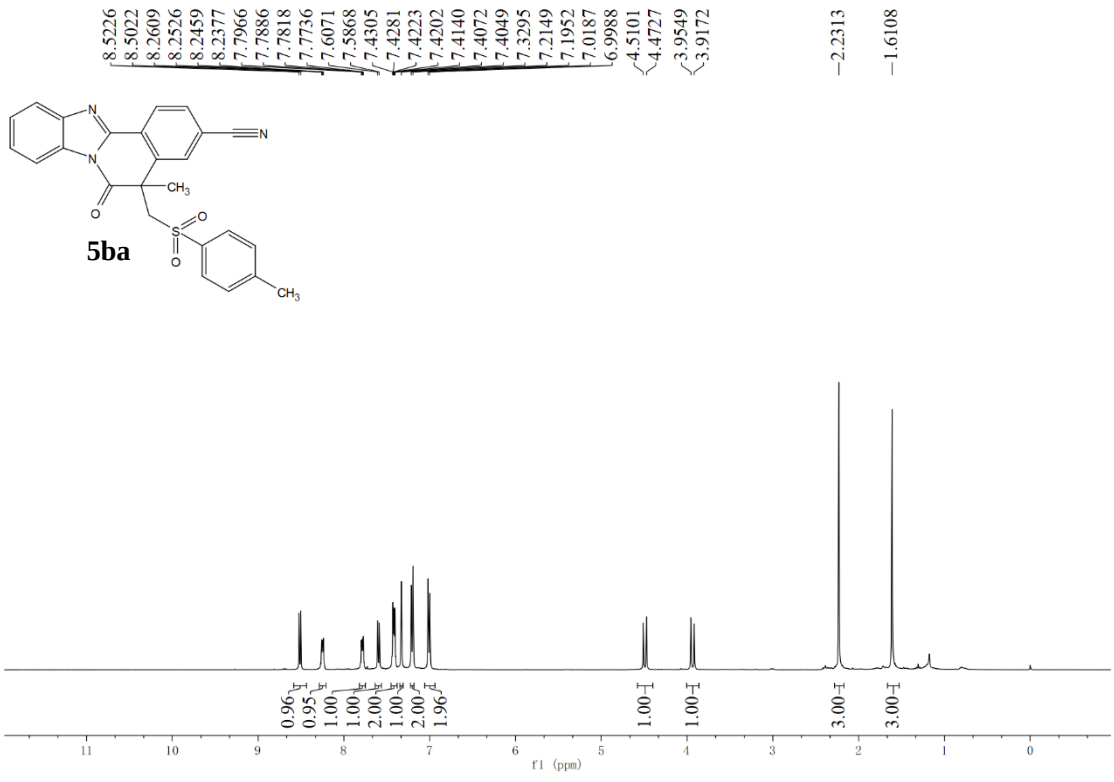
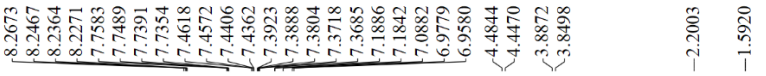
0.95
1.00
5.03
1.03
2.04
0.99
0.96
0.99
3.00
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


8.4424
8.4228
8.2523
8.2469
8.2348
8.2299
7.7839
7.7793
7.7679
7.7623
7.4963
7.4746
7.4662
7.4453
7.4071
7.4032
7.3955
7.3900
7.3831
7.3765
7.3728
7.3625
7.3438
7.1882
7.1724
7.1531
7.1343
7.0576
4.5273
4.4901
3.9969
3.9596
1.6255
0.95
0.95
1.00
7.00
1.27
1.00
1.00
1.00
3.00
f1 (ppm)

5ak


8.5226
8.5022
8.2609
8.2526
8.2459
8.2377
7.7966
7.7886
7.7818
7.7736
7.6071
7.5868
7.4305
7.4281
7.4223
7.4202
7.4140
7.4072
7.4049
7.3295
7.2149
7.1952
7.0187
6.9988
4.5101
4.4727
3.9549
3.9172
2.2313
1.6108
0.96
0.95
1.00
1.00
2.00
1.00
2.00
1.96
1.00
1.00
3.00
3.00
f1 (ppm)

5ba


8.2673
8.2467
8.2364
8.2271
7.7583
7.7489
7.7391
7.7354
7.4618
7.4572
7.4406
7.4362
7.3923
7.3888
7.3804
7.3718
7.3685
7.1886
7.1842
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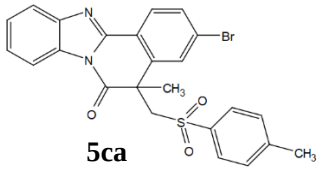
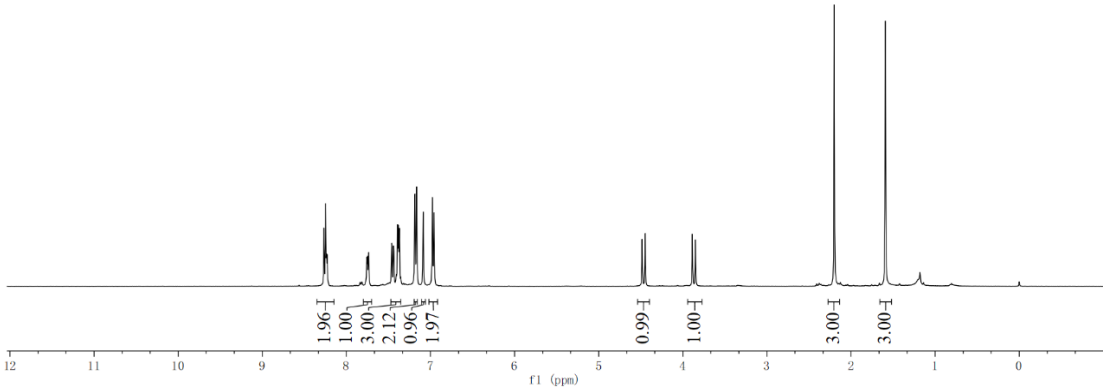
6.9779
6.9580
4.4844
4.4470
3.8872
3.8498
2.2003
1.5920


N
N
Br
CH3
O
O
S
O
CH3

5ca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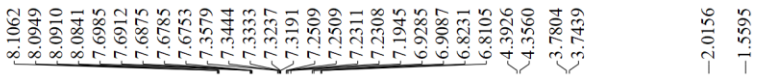
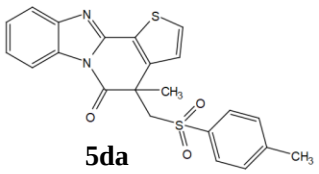
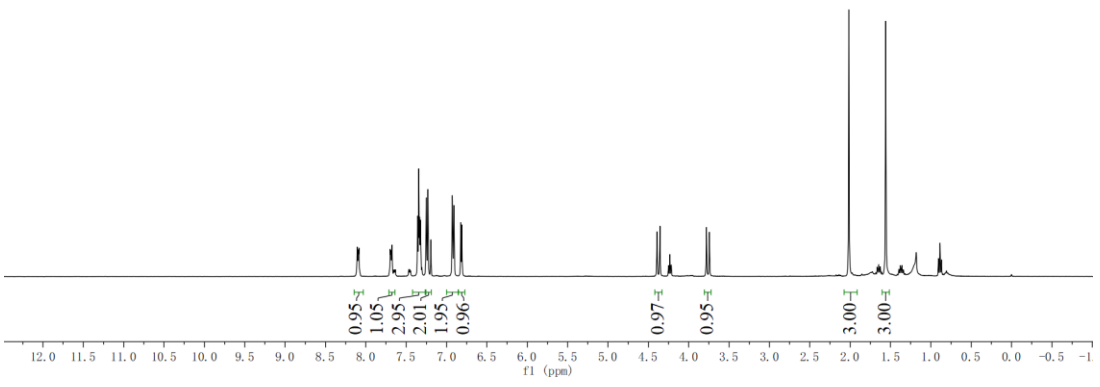
1.00
3.00
2.12
0.96
1.97
0.99
1.00
3.00
3.00
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


8.1062
8.0949
8.0910
8.0841
7.6985
7.6912
7.6875
7.6785
7.6753
7.3579
7.3444
7.3333
7.3237
7.3191
7.2509
7.2509
7.2311
7.2308
7.1945
6.9285
6.9087
6.8231
6.8105
4.3926
4.3560
3.7804
3.7439
2.0156
1.5595


N
N
S
CH3
O
O
S
O
CH3

5da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1.05
2.95
2.01
1.95
0.96
0.97
0.95
3.00
3.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)